

Inventory (please provide full name): _____

Earliest Priority Date: _____

Search Topic:

Please provide a concise description of the invention, including the nature of the problem to be solved, the solution proposed, and the advantages of the invention. Include a brief description of the structure of the invention, and a brief description of the method of use.

*For claims of Structure Only: Please provide an accurate description of the structure, including the nature of the problem to be solved, the solution proposed, and the advantages of the invention.

See claims attached. Please do structure, name, and inventory name(s). Please. Display results to show identification of source, and F.R. ⁴⁰ compound nearest structure of identified compounds. Search compounds of Formula III as indicated. See previous searches.

Please call with any questions

STAFF USE ONLY

Type of Search:

Number and date when completed:

Searcher: _____

No. required:_____
Date:

Date of Search:

No. required:_____
Date:

Number of Results:

No. required:_____
Date:

Date of Search:

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No. required:_____
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L1 1 SEA FILE=HCAPLUS SPE=ON ABB=ON PLU=ON US2004-772445/APPS

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YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS' - CONTINUE? (Y)/N:y

L1 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:576785 HCAPLUS Full-text

DOCUMENT NUMBER: 131:214294

TITLE: Preparation of substituted quinazolines and heterocyclic analogs as antagonists or positive modulators of AMPA receptors

INVENTOR(S): Upasani, Ravi; Cai, Sui X.; Lan, Nancy C.; Wang, Yan; Field, George; Fick, David B.

PATENT ASSIGNEE(S): Cocosys, Inc., USA

SOURCE: PCT Int. Appl., 117 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

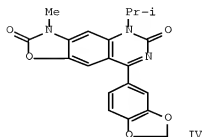
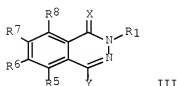
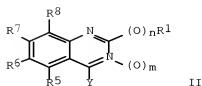
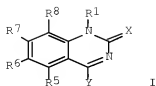
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|--------------|
| WO 9944612 | A1 | 19990910 | WO 1999-US4609 | 19990302 |
| W: JP, US | | | | |
| RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| EP 1066039 | A1 | 20010110 | EP 1999-911063 | 19990302 |
| R: BE, CH, DE, ES, FR, GB, IT, LI, NL, IE | | | | |
| JP 2002505288 | T | 20020219 | JP 2000-534214 | 19990302 |
| US 6465472 | B1 | 20021015 | US 2000-654839 | 20000901 |
| US 20030033089 | A1 | 20030213 | US 2002-219755 | 20020816 |
| US 6765006 | B2 | 20040720 | | |
| US 20040162299 | A1 | 20040819 | US 2004-772445 | 20040206 <-- |
| PRIORITY APPLN. INFO.: | | | US 1998-76451P | P 19980302 |
| | | | WO 1999-US4609 | W 19990302 |
| | | | US 2000-654839 | A3 20000901 |
| | | | US 2002-219755 | A3 20020816 |

OTHER SOURCE(S): MARPAT 131:214294

ED Entered STN: 14 Sep 1999

GI



AB Substituted quinazolines and heterocyclic analogs (I, II, and III) [R1 = (un)substituted alkyl, alkenyl, or alkynyl; R5 and R8 = independently H, halogen, NO2, NH2, CN, alkanoylamido, OH, SH, alkoxy, (un)substituted alkyl, (hetero)aryl, heterocyclic, alkenyl, or alkynyl, etc.; R6 and R7 taken together = 5- or 6-membered carbocyclic or heterocyclic ring; X = O or S; Y = (hetero)aryl; n and m = independently 0 or 1] were prepared as antagonists or pos. modulators of AMPA receptors for treatment, prevention, or amelioration of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia. Thus, 3-methyl-5-nitro-2(3H)-benzoxazolone was reduced to the amine over Pt/C in glacial acetic acid. Na cyanoborohydride was added to a suspension of the amine, THF, acetic acid, and acetone followed by treatment with NaOH and water to precipitate 5-(isopropylamino)-3-methyl-2(3H)-benzoxazolone. The substituted amine was converted to the ureido derivative by stirring with KCNO in glacial acetic acid for 5 days. The urea was cyclized with piperonal in benzene and methanesulfonic acid to form the 3,4-dihydrooxazolo[4,5-g]quinazolin-2(1H)-one. The product was reduced by addition of KMnO4 in H2O followed by treatment with formalin to yield 1-isopropyl-4-(3,4-methylenedioxiphenyl)-8-methyl-7-oxoxazolo[4,5-g]quinazolin-2(1H)-one (IV). Selected compds. of the invention were tested for preferred binding to AMPA receptors and exhibited IC50 values ranging from 0.2 to 13 μ M. The anticonvulsant activity of the AMPA antagonists was evaluated in the Maximal Electroshock-induced Seizure (MES) test. MES ED50 values ranged from 1 to 10 mg/kg i.v.

IC ICM A61K031-50

ICS A61K031-505; C07D237-26; C07D239-70; C07D491-04; C07D491-048;
C07D491-056; C07D498-04

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1

ST quinazoline AMPA receptor antagonist pos modulator prepn; ischemia amyotrophic lateral sclerosis schizophrenia treatment quinazoline prepn; anticonvulsant quinazoline prepn; analgesic quinazoline prepn; excitatory amino acid neurotransmitter antagonist quinazoline prepn; learning cognition enhancer quinazoline prepn

IT Glutamate receptors

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(AMPA-binding, agonists; preparation of substituted quinazolines and

- heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)
- IT Nervous system
(amyotrophic lateral sclerosis, treatment; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)
- IT Nerve
Nervous system
(degeneration, treatment; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)
- IT Neurotransmitter antagonists
(excitatory amino acid; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)
- IT Heart, disease
(ischemia, treatment; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)
- IT Cytoprotective agents
(neuroprotectants; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)
- IT Analgesics
Anti-ischemic agents
Anticonvulsants
Cognition enhancers
Glutamate agonists
(preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)
- IT Schizophrenia
(treatment; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)
- IT 85575-56-0P 99584-09-5P 243134-92-1P 243134-93-2P 243134-94-3P
243134-95-4P 243134-96-5P 243134-97-6P 243134-98-7P 243134-99-8P
243135-00-4P 243135-01-5P 243135-02-6P 243135-03-7P 243135-04-8P
243135-05-9P 243135-06-0P 243135-07-1P 243135-08-2P 243135-09-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)
- IT 243135-42-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of substituted quinazolines and heterocyclic analogs as

antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)

| | | | | | |
|----|-------------|-------------|-------------|-------------|-------------|
| IT | 243135-18-4 | 243135-19-5 | 243135-20-8 | 243135-21-9 | 243135-22-0 |
| | 243135-23-1 | 243135-24-2 | 243135-25-3 | 243135-26-4 | 243135-27-5 |
| | 243135-28-6 | 243135-29-7 | 243135-30-0 | 243135-31-1 | 243135-32-2 |
| | 243135-33-3 | 243135-34-4 | 243135-35-5 | 243135-36-6 | 243135-37-7 |
| | 243135-38-8 | 243135-39-9 | 243135-40-2 | 243135-41-3 | |

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)

| | | |
|----|--|--|
| IT | 60-56-0, 2-Mercapto-1-methylimidazole | 66-99-9, 2-Naphthaldehyde |
| | 67-64-1, 2-Propanone, reactions | 75-30-9, 2-Iodopropane |
| | 100-10-7, 4-(Dimethylamino)benzaldehyde | 100-39-0, Benzyl bromide |
| | 100-52-7, Benzaldehyde, reactions | 110-85-0, Piperazine, reactions |
| | 115-80-0, Triethyl orthopropionate | 120-57-0, Piperonal |
| | 123-75-1, Pyrrolidine, reactions | 288-32-4, Imidazole, reactions |
| | 500-22-1, 3-Pyridinecarboxaldehyde | 656-42-8 |
| | 1544-85-0, 5-Amino-2,2-difluoro-1,3-benzodioxole | 3218-36-8, 4-Phenylbenzaldehyde |
| | 3889-13-2 | 4584-46-7, 2-(Dimethylamino)ethyl chloride hydrochloride |
| | 7051-34-5, (Bromomethyl)cyclopropane | 13669-42-6, 3-Quinolonecarboxaldehyde |
| | 14268-66-7, 3,4-(Methylenedioxy)aniline | 15952-61-1, 6-Chloropiperonal |
| | 16081-45-1, 5-Amino-1,4-benzodioxane | 22013-33-8, 1,4-Benzodioxan-6-amine |
| | 24425-40-9 | 25054-53-9, Piperonyl chloride |
| | 29668-44-8, 1,4-Benzodioxan-6-carboxaldehyde | 30084-91-4, 5-Indancarboxaldehyde |
| | 32953-14-3, N-Ethyl-3,4-(methylenedioxy)aniline | 94614-83-2 |
| | 101084-60-0 | 109258-03-9 |
| | 243135-10-6 | 243135-11-7 |
| | 243135-12-8 | 243135-13-9 |
| | 243135-14-0 | 243135-15-1 |
| | 243135-16-2 | 243135-17-3 |

RL: RCT (Reactant); RACT (Reactant or reagent)

(reactant; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)

| | | | | | |
|----|--------------|--------------|--------------|--------------|--------------|
| IT | 10368-14-6P | 33095-75-9P | 33095-79-3P | 33095-82-8P | 33095-94-2P |
| | 34060-22-5P | 40484-04-6P | 59856-06-3P | 63546-19-0P | 85575-57-1P |
| | 164526-15-2P | 243133-76-8P | 243133-77-9P | 243133-78-0P | 243133-79-1P |
| | 243133-81-5P | 243133-82-6P | 243133-85-9P | 243133-86-0P | 243133-88-2P |
| | 243133-90-6P | 243133-92-8P | 243133-94-0P | 243133-95-1P | 243133-96-2P |
| | 243133-97-3P | 243133-98-4P | 243133-99-5P | 243134-07-8P | 243134-13-6P |
| | 243134-40-9P | 243134-48-7P | 243134-49-8P | 243134-53-4P | 243134-58-9P |
| | 243134-66-9P | 243134-73-8P | | | |

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(target compound; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)

| | | | | | |
|----|--------------|--------------|--------------|--------------|--------------|
| IT | 13067-19-1P | 33095-76-0P | 33100-29-7P | 40483-99-6P | 119179-46-3P |
| | 243133-80-4P | 243133-83-7P | 243133-84-8P | 243133-87-1P | 243133-89-3P |
| | 243133-91-7P | 243133-93-9P | 243134-00-1P | 243134-01-2P | 243134-02-3P |
| | 243134-03-4P | 243134-04-5P | 243134-05-6P | 243134-06-7P | 243134-08-9P |
| | 243134-09-0P | 243134-10-3P | 243134-11-4P | 243134-12-5P | 243134-14-7P |
| | 243134-15-8P | 243134-16-9P | 243134-17-0P | 243134-18-1P | 243134-19-2P |

| | | | | |
|--------------|--------------|--------------|--------------|--------------|
| 243134-20-5P | 243134-21-6P | 243134-22-7P | 243134-23-8P | 243134-24-9P |
| 243134-25-0P | 243134-26-1P | 243134-27-2P | 243134-28-3P | 243134-29-4P |
| 243134-30-7P | 243134-31-8P | 243134-32-9P | 243134-33-0P | 243134-34-1P |
| 243134-35-2P | 243134-36-3P | 243134-37-4P | 243134-38-5P | 243134-42-1P |
| 243134-44-3P | 243134-46-5P | 243134-50-1P | 243134-51-2P | 243134-52-3P |
| 243134-54-5P | 243134-55-6P | 243134-56-7P | 243134-57-8P | 243134-59-0P |
| 243134-60-3P | 243134-61-4P | 243134-62-5P | 243134-63-6P | 243134-64-7P |
| 243134-65-8P | 243134-67-0P | 243134-68-1P | 243134-69-2P | 243134-70-5P |
| 243134-71-6P | 243134-72-7P | 243134-74-9P | 243134-75-0P | 243134-76-1P |
| 243134-77-2P | 243134-78-3P | 243134-79-4P | 243134-80-7P | 243134-81-8P |
| 243134-82-9P | 243134-83-0P | 243134-84-1P | 243134-85-2P | 243134-86-3P |
| 243134-87-4P | 243134-88-5P | 243134-89-6P | 243134-90-9P | 243134-91-0P |

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(target compound; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L2 1 SEA FILE=WPIX SPE=ON ABB=ON PLU=ON US2004-772445/APPS

=> d iall code 12

YOU HAVE REQUESTED DATA FROM FILE 'WPIX' - CONTINUE? (Y)/N:y

L2 ANSWER 1 OF 1 WPIX COPYRIGHT 2008 THOMSON REUTERS on STN
ACCESSION NUMBER: 1999-540736 [45] WPIX
DOC. NO. CPI: C1999-157966 [45]
TITLE: Substituted quinazolines and pharmaceutically acceptable salts and prodrugs as alpha-amino-3-hydroxy-5-methylisoxazole-4-propionic acid receptor modulators - used to treat neuronal loss associated with stroke and neurodegenerative diseases B02
DERWENT CLASS: CAI S X; FICK D B; FIELD G; LAN N C; UPASANI R; WANG Y
INVENTOR: (COCE-N) COCENSYS INC; (EURO-N) EUROCELTIQUE SA
PATENT ASSIGNEE:
COUNTRY COUNT: 21

PATENT INFORMATION:

| PATENT NO | KIND DATE | WEEK | LA | PG | MAIN IPC |
|----------------|-------------|-----------|----|--------|----------|
| WO 9944612 | A1 19990910 | (199945)* | EN | 117[0] | |
| EP 1066039 | A1 20010110 | (200103) | EN | | |
| JP 2002505288 | W 20020219 | (200216) | JA | 142 | |
| US 6465472 | B1 20021015 | (200271) | EN | | |
| US 20030033089 | A1 20030213 | (200314) | EN | | |
| US 6765006 | B2 20040720 | (200448) | EN | | |
| US 20040162299 | A1 20040819 | (200455) | EN | | |

APPLICATION DETAILS:

| PATENT NO | KIND | APPLICATION | DATE |
|-------------------|-------------|-----------------------|-----------------|
| WO 9944612 A1 | | WO 1999-US4609 | 19990302 |
| US 6465472 B1 | Provisional | US 1998-76451P | 19980302 |
| US 20030033089 A1 | Provisional | US 1998-76451P | 19980302 |
| US 6765006 B2 | Provisional | US 1998-76451P | 19980302 |
| US 20040162299 A1 | Provisional | US 1998-76451P | 19980302 |
| EP 1066039 A1 | | EP 1999-911063 | 19990302 |
| EP 1066039 A1 | | WO 1999-US4609 | 19990302 |
| JP 2002505288 W | | WO 1999-US4609 | 19990302 |
| US 6465472 B1 | Cont of | WO 1999-US4609 | 19990302 |
| US 20030033089 A1 | Cont of | WO 1999-US4609 | 19990302 |
| US 6765006 B2 | Cont of | WO 1999-US4609 | 19990302 |
| US 20040162299 A1 | Cont of | WO 1999-US4609 | 19990302 |
| JP 2002505288 W | | JP 2000-534214 | 19990302 |
| US 6465472 B1 | | US 2000-654839 | 20000901 |
| US 20030033089 A1 | Div Ex | US 2000-654839 | 20000901 |
| US 20040162299 A1 | Div Ex | US 2000-654839 | 20000901 |
| US 6765006 B2 | Div Ex | US 2001-654839 | 20010901 |
| US 20030033089 A1 | | US 2002-219755 | 20020816 |
| US 6765006 B2 | | US 2002-219755 | 20020816 |
| US 20040162299 A1 | Div Ex | US 2002-219755 | 20020816 |
| US 20040162299 A1 | | <u>US 2004-772445</u> | <u>20040206</u> |

FILING DETAILS:

| PATENT NO | KIND | PATENT NO |
|-------------------|----------|--------------|
| US 20030033089 A1 | Div ex | US 6465472 B |
| US 6765006 B2 | Div ex | US 6465472 B |
| US 20040162299 A1 | Div ex | US 6465472 B |
| EP 1066039 A1 | Based on | WO 9944612 A |
| JP 2002505288 W | Based on | WO 9944612 A |

PRIORITY APPLN. INFO: US 1998-76451P 19980302
 WO 1999-US4609 19990302
 US 2000-654839 20000901
 US 2001-654839 20010901
 US 2002-219755 20020816
US 2004-772445 20040206

INT. PATENT CLASSIF.:

MAIN: C07D491-056

INDEX: C07D239:80; C07D317:10

IPC RECLASSIF.: A61K0031-502 [I,A]; A61K0031-502 [I,C]; A61K0031-5025 [I,A]; A61K0031-5025 [I,C]; A61K0031-517 [I,A]; A61K0031-517 [I,C]; A61K0031-519 [I,A]; A61K0031-519 [I,C]; A61P0025-00 [I,C]; A61P0025-08 [I,A]; A61P0025-18 [I,A]; A61P0025-28 [I,A]; A61P0009-00 [I,C]; A61P0009-10 [I,A]; C07D0237-00 [I,C]; C07D0237-32 [I,A]; C07D0239-00 [I,C]; C07D0239-82 [I,A]; C07D0405-00 [I,C]; C07D0405-04 [I,A]; C07D0491-00 [I,C]; C07D0491-04 [I,A]; C07D0491-048 [I,A]; C07D0491-056 [I,A]; C07D0498-00 [I,C]; C07D0498-04 [I,A]; C07D0521-00 [I,A]; C07D0521-00 [I,C]

ECLA: C07D0239-82; C07D0491-04+317A+237A;
 C07D0491-04+317A+239A; C07D0491-04+319A+239A;
 C07D0498-04+263A+239A; C07D0521-00B1C8

ICO: M07D0239:82
 USCLASS NCLM: 514/232.800

NCLS: 514/266.310; 514/267.000; 544/115.000; 544/250.000;
544/284.000; 544/286.000

BASIC ABSTRACT:

WO 1999044612 A1 UPAB: 20060503

NOVELTY - Substituted quinazolines and their pharmaceutically acceptable salts and prodrugs.

DETAILED DESCRIPTION - Substituted quinazolines are of formula (I):

R1 = alkyl, haloalkyl, aminoalkyl, alkenyl, alkynyl, aralkyl, aralkenyl, aralkynyl, heteroaralkyl, carbocycloalkyl, heterocycloalkyl, hydroxyalkyl, cyanoalkyl, alkanoylamidoalkyl, alkanoyloxyalkyl, azidoalkyl, alkenyloxyalkyl or alkoxyalkyl;

R6, R7 taken together = 5-6-membered carbocyclic or heterocyclic ring;

R5, R8 = H, halo, haloalkyl, aryl, heterocycle, heteroaryl, alkyl, alkenyl, alkynyl, aralkyl, aralkenyl, aralkynyl, hydroxyalkyl, nitro, amino, cyano, alkanoylamido, hydroxy, thiol, alkanoyloxy, alkoxy, carboxy, carbonylamido or thioalkoxy;

X = O or S; and

Y = aryl or heteroaryl.

INDEPENDENT CLAIMS are also included for:

- (1) compounds of formula (II);
- (2) compounds of formula (III)

n, z = 0-1.

ACTIVITY - Neuroprotective; neuroregenerative; anxiolytic; anti-psychotic; anticonvulsant; analgesic; anti-migraine; anti-glaucoma; anti-retinitis; anti-urinary incontinence; anesthetic; cognitive improving; anti-schizophrenia; anti-mycobionus.

MECHANISM OF ACTION - Alpha-amino-3-hydroxy-5-methylisoxazole-4-propionic acid (AMPA) ionotropic receptor antagonists; AMPA positive modulators.

USE - Used to treat, prevent or ameliorate neuronal loss associated with stroke, ischemia including global ischemia especially as a result of cardiac arrest, CNS trauma, hypoglycemia or surgery, to treat or ameliorate neurodegenerative diseases including Alzheimer's disease, amyotrophic lateral sclerosis, Huntington's disease, Parkinson's disease and Down's syndrome, to treat, prevent or ameliorate adverse consequences of the overstimulation of excitatory amino acids, to treat, prevent or ameliorate anxiety, psychosis, convulsions, chronic pain, migraine headache, glaucoma, retinitis and urinary incontinence, to induce anesthesia, to enhance learning and cognition, to treat or ameliorate schizophrenia or myoclonus (claimed). Also used to treat acute neurological disorders such as domoic acid poisoning, cerebral ischemia, stroke, spinal cord trauma, hypoxia, anoxia, carbon monoxide, cyanide or manganese poisoning, hypoglycemia, mechanical trauma to the nervous system, neuronal injury associated with HIV and AIDS, AIDS dementia, neuropathic pain syndrome, olivopontocerebral atrophy, mitochondrial abnormalities, hepatic encephalopathy, Tourette's syndrome, drug addiction, acute and chronic pain, pain associated with post-therapeutic neuralgia, interstitial cystitis, osteoarthritis, spinal cord injury, diabetic neuropathy, generalized anxiety disorder, phobic disorders, obsessive-compulsive disorders, panic disorders and post-traumatic stress disorder.

MANUAL CODE:

CPI: B06-E05; B14-C01; B14-C09A; B14-F01; B14-F01B;
B14-F02D1; B14-J01A3; B14-J01A4; B14-J01B3; B14-J01B4;
B14-J07; B14-M01C; B14-N03; B14-N07D; B14-N16; B14-S01

AN 1999-540736 [45] WPIX

DC B02

IC ICM C07D491-056

ICI C07D239:80; C07D317:10

IPCR A61K0031-502 [I,A]; A61K0031-502 [I,C]; A61K0031-5025 [I,A]; A61K0031-5025 [I,C]; A61K0031-517 [I,A]; A61K0031-517 [I,C]; A61K0031-519 [I,A]; A61K0031-519 [I,C]; A61P0025-00 [I,C]; A61P0025-08 [I,A]; A61P0025-16 [I,A]; A61P0025-18 [I,A]; A61P0025-28 [I,A]; A61P0009-00 [I,C]; A61P0009-10 [I,A]; C07D0237-00 [I,C]; C07D0237-32 [I,A]; C07D0239-00

[I,C]; C07D0239-82 [I,A]; C07D0405-00 [I,C]; C07D0405-04 [I,A];
C07D0491-00 [I,C]; C07D0491-04 [I,A]; C07D0491-048 [I,A]; C07D0491-056
[I,A]; C07D0498-00 [I,C]; C07D0498-04 [I,A]; C07D0521-00 [I,A];
C07D0521-00 [I,C]

EPC C07D0239-82; C07D0491-04+317A+237A; C07D0491-04+317A+239A;
C07D0491-04+319A+239A; C07D0498-04+263A+239A; C07D0521-00B1C8

ICO M07D0239:82

NCL NCLM 514/232.800
NCLS 514/266.310; 514/267.000; 544/115.000; 544/250.000; 544/284.000;
544/286.000

IT UPIT 20060503
232212-CL 232212-NEW; 232213-CL 232213-NEW; 232214-CL 232214-NEW;
232215-CL 232215-NEW; 232216-CL 232216-NEW; 232217-CL 232217-NEW;
232218-CL 232218-NEW; 232219-CL 232219-NEW; 232220-CL 232220-NEW;
232874-CL 232874-NEW; 232875-CL 232875-NEW; 232876-CL 232876-NEW;
232877-CL 232877-NEW; 232878-CL 232878-NEW; 232879-CL 232879-NEW;
232880-CL 232880-NEW; 232881-CL 232881-NEW; 0006-89701-CL 0006-89701-NEW;
0006-89702-CL 0006-89702-NEW; 0006-89703-CL 0006-89703-NEW

MC CPI: B06-E05; B14-C01; B14-C09A; B14-F01; B14-F01B; B14-F02D1; B14-J01A3;
B14-J01A4; B14-J01B3; B14-J01B4; B14-J07; B14-M01C; B14-N03;
B14-N07D; B14-N16; B14-S01

CMC UPB 20060503
M2 *01* D014 E530 G021 H2 H211 J5 J521 L9 L921 M1 M115 M210 M212
M273 M281 M320 M412 M511 M520 M531 M540 M710 P411 P412 P421 P440
P442 P446 P522 P625 P646 M905 M904
RIN: 02803
DCN: RA0040-N RA0040-T
DCR: 232212-N 232212-T

M2 *02* J5 J521 L9 L921 M1 M115 M210 M213 M232 M273 M281 M320 M412 M511
M520 M531 M540 M710 P411 P412 P421 P440 P442 P446 P522 P625 P646
M905 M904
RIN: 02803
DCN: RA0041-N RA0041-T
DCR: 232213-N 232213-T

M2 *03* D014 D022 D140 E530 G030 G530 H2 H211 J5 J521 L9 L921 M1 M115
M280 M311 M321 M342 M373 M391 M412 M512 M520 M710 P411 P412 P421
P440 P442 P446 P522 P625 P646 M905
RIN: 02803
DCN: RA0042-N RA0042-T
DCR: 232214-N 232214-T

M2 *04* D014 D022 D140 E530 H1 H103 H181 H2 H211 J5 J521 L9 L921 M1 M115
M210 M212 M273 M282 M312 M321 M332 M342 M383 M391 M412 M512 M520
M530 M540 M710 P411 P412 P421 P440 P442 P446 P522 P625 P646
M905 M904
RIN: 02803
DCN: RA0043-N RA0043-T
DCR: 232215-N 232215-T

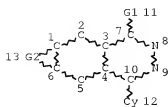
M2 *05* D014 D022 D140 E530 H2 H211 H7 H731 J5 J521 L9 L921 M1 M115 M210
M213 M231 M273 M281 M320 M412 M512 M520 M530 M540 M710 P411 P412
P421 P440 P442 P446 P522 P625 P646 M905 M904
RIN: 02803
DCN: RA0044-N RA0044-T
DCR: 232216-N 232216-T

M2 *06* D013 D022 D140 E530 H1 H103 H181 H5 H521 H8 L921 M1 M115 M210
M212 M273 M282 M312 M321 M332 M342 M383 M391 M412 M512 M520 M530
M540 M710 P411 P412 P421 P440 P442 P446 P522 P625 P646 M905
M904
RIN: 02803
DCN: RA0045-N RA0045-T
DCR: 232217-N 232217-T

M2 *07* D013 D022 D140 E530 H1 H103 H181 H5 H521 H8 L921 M1 M115 M210
 M211 M273 M282 M312 M321 M332 M342 M383 M391 M412 M512 M520 M530
 M540 M710 P411 P412 P421 P440 P442 P446 P522 P625 P646 M905
 M904
 RIN: 02803
 DCN: RA0046-N RA0046-T
 DCR: 232218-N 232218-T
 M2 *08* D013 D022 D140 E530 H1 H100 H181 H5 H521 H8 L921 M1 M115 M280
 M312 M321 M332 M342 M383 M391 M412 M512 M520 M530 M540 M710 P411
 P412 P421 P440 P442 P446 P522 P625 P646 M905 M904
 RIN: 02803
 DCN: RA0047-N RA0047-T
 DCR: 232219-N 232219-T
 M2 *09* D013 D022 D140 E530 F011 F423 H1 H181 H2 H201 H5 H521 H8 L921 M1
 M115 M280 M312 M321 M332 M342 M383 M391 M412 M512 M521 M530 M540
 M710 P411 P412 P421 P440 P442 P446 P522 P625 P646 M905 M904
 RIN: 02803
 DCN: RA0048-N RA0048-T
 DCR: 232220-N 232220-T
 M2 *10* D014 D022 D140 E530 H2 H211 J0 J011 J2 J271 J5 J521 L9 L941 M1
 M115 M210 M212 M272 M281 M312 M321 M332 M342 M383 M391 M412 M512
 M520 M530 M540 M710 P411 P412 P421 P440 P442 P446 P522 P625 P646
 M905 M904
 RIN: 02805
 DCN: RA00N1-N RA00N1-T
 DCR: 232874-N 232874-T
 M2 *11* D014 D022 D140 E530 F011 F423 H1 H181 H2 H201 H211 J5 J521 L9
 L941 M1 M115 M280 M312 M321 M332 M342 M383 M391 M412 M512 M521
 M530 M540 M710 P411 P412 P421 P440 P442 P446 P522 P625 P646
 M905 M904
 RIN: 02805
 DCN: RA00N2-N RA00N2-T
 DCR: 232875-N 232875-T
 M2 *12* D014 D022 D140 E530 F011 F433 H1 H181 H2 H201 H211 J5 J521 L9
 L941 M1 M115 M280 M312 M321 M332 M342 M383 M391 M412 M512 M521
 M530 M540 M710 P411 P412 P421 P440 P442 P446 P522 P625 P646
 M905 M904
 RIN: 02805
 DCN: RA00N3-N RA00N3-T
 DCR: 232876-N 232876-T
 M2 *13* D013 D022 D140 E530 J5 J521 L9 L941 M1 M115 M280 M320 M412 M512
 M520 M530 M540 M710 P411 P412 P421 P440 P442 P446 P522 P625 P646
 M905 M904
 RIN: 02805
 DCN: RA00N4-N RA00N4-T
 DCR: 232877-N 232877-T
 M2 *14* D014 D022 D140 E530 F011 F521 H1 H181 H2 H201 H211 J5 J521 L9
 L941 M1 M115 M280 M312 M321 M332 M342 M383 M391 M412 M512 M521
 M530 M540 M710 P411 P412 P421 P440 P442 P446 P522 P625 P646
 M905 M904
 RIN: 02805
 DCN: RA00N5-N RA00N5-T
 DCR: 232878-N 232878-T
 M2 *15* D014 D022 D140 E530 H2 H211 J5 J521 L9 L941 M1 M115 M210 M212
 M273 M281 M320 M412 M512 M520 M530 M540 M710 P411 P412 P421 P440
 P442 P446 P522 P625 P646 M905 M904
 RIN: 02805
 DCN: RA00N6-N RA00N6-T
 DCR: 232879-N 232879-T
 M2 *16* M1 M115 M210 M211 M273 M282 M312 M321 M332 M342 M383 M391 M412

M512 M520 M530 M540 M710 P411 P412 P421 P440 P442 P446 P522 P625
 P646 M905 M904
 RIN: 02805
 DCN: RA00N7-N RA00N7-T
 DCR: 232880-N 232880-T
 M2 *17* D014 D022 D140 E530 H1 H103 M710 P411 P412 P421 P440 P442 P446
 P522 P625 P646 M905
 RIN: 02805
 DCN: RA00N8-N RA00N8-T
 DCR: 232881-N 232881-T
 M2 *18* D014 D021 D023 D040 F010 F019 F020 F021 F029 G010 G019 G020 G021
 G029 G030 G040 G050 G100 G111 G112 G113 G221 G299 G553 G563 H100
 H101 H141 H142 H181 H2 H211 H341 H342 H401 H402 H403 H441 H442
 H481 H482 H483 H494 H498 H541 H542 H600 H608 H609 H641 H642 H681
 H682 H683 H689 H713 H715 H716 H721 H722 H723 H731 J011 J012 J013
 J131 J132 J241 J242 J341 J342 J371 J5 J521 J592 L143 L145 L199
 L640 L650 L699 L9 L921 L922 M1 M112 M113 M114 M115 M116 M119
 M122 M124 M129 M132 M135 M139 M150 M210 M211 M212 M213 M214 M215
 M216 M220 M221 M222 M223 M224 M225 M226 M231 M232 M233 M240 M262
 M272 M273 M280 M281 M282 M283 M311 M312 M313 M314 M315 M316 M320
 M321 M322 M323 M331 M332 M333 M334 M340 M342 M343 M344 M349 M353
 M362 M373 M381 M383 M391 M392 M393 M412 M511 M520 M521 M522 M523
 M530 M531 M532 M533 M540 M541 M710 P411 P412 P421 P440 P442 P446
 P522 P625 P646 M905 M904
 MCN: 0006-89701-N 0006-89701-T
 M2 *19* D014 D021 D023 D040 F010 F019 F020 F021 F029 G010 G019 G020 G021
 G029 G030 G040 G050 G100 G111 G112 G113 G221 G299 G553 G563 H100
 H101 H141 H142 H181 H2 H211 H341 H342 H401 H402 H403 H441 H442
 H481 H482 H483 H494 H498 H541 H542 H600 H608 H609 H641 H642 H681
 H682 H683 H689 H713 H715 H716 H721 H722 H723 H731 J011 J012 J013
 J131 J132 J241 J242 J341 J342 J371 J5 J521 J592 L143 L145 L199
 L640 L650 L699 L9 L941 L943 M1 M112 M113 M114 M115 M116 M119
 M122 M124 M129 M132 M135 M139 M150 M210 M211 M212 M213 M214 M215
 M216 M220 M221 M222 M223 M224 M225 M226 M231 M232 M233 M240 M262
 M272 M273 M280 M281 M282 M283 M311 M312 M313 M314 M315 M316 M320
 M321 M322 M323 M331 M332 M333 M334 M340 M342 M343 M344 M349 M353
 M362 M373 M381 M383 M391 M392 M393 M412 M511 M520 M521 M522 M523
 M530 M531 M532 M533 M540 M541 M710 P411 P412 P421 P440 P442 P446
 P522 P625 P646 M905 M904
 MCN: 0006-89702-N 0006-89702-T
 M2 *20* D013 D014 D021 D023 D040 F010 F019 F020 F021 F029 G010 G019 G020
 G021 G029 G030 G040 G050 G100 G111 G112 G113 G221 G299 G553 G563
 H100 H101 H141 H142 H181 H341 H342 H401 H402 H403 H441 H442 H481
 H482 H483 H494 H498 H521 H541 H542 H600 H608 H609 H641 H642 H681
 H682 H683 H689 H715 H721 H722 H723 H731 J011 J012 J013 J131 J132
 J241 J242 J341 J342 J371 K850 L143 L145 L199 L640 L650 L660 L699
 L921 M1 M112 M113 M114 M115 M116 M119 M122 M123 M124 M125 M126
 M129 M132 M135 M139 M141 M150 M210 M211 M212 M213 M214 M215 M216
 M220 M221 M222 M223 M224 M225 M226 M231 M232 M233 M240 M262 M272
 M280 M281 M282 M283 M311 M312 M313 M314 M315 M316 M320 M321 M322
 M323 M331 M332 M333 M334 M340 M342 M343 M344 M349 M353 M362 M372
 M373 M381 M383 M391 M392 M393 M412 M511 M520 M521 M522 M523 M530
 M531 M532 M533 M540 M541 M710 P411 P412 P421 P440 P442 P446 P522
 P625 P646 M905 M904
 MCN: 0006-89703-N 0006-89703-T

```
=> => d que stat 110
L8          STR
```



```
O @14      S @15
```

```
VAR G1=14/15
REP G2=(1-6) A
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 14
CONNECT IS E1 RC AT 15
DEFAULT MLEVEL IS ATOM
GGCAT IS UNS AT 12
DEFAULT ECLEVEL IS LIMITED
```

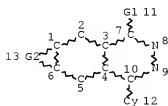
```
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 15
```

```
STEREO ATTRIBUTES: NONE
L10          56 SEA FILE=REGISTRY SSS FUL L8
```

```
100.0% PROCESSED 83282 ITERATIONS
SEARCH TIME: 00.00.04
```

```
56 ANSWERS
```

```
=> d que stat 115
L8          STR
```



```
O @14      S @15
```

```
VAR G1=14/15
REP G2=(1-6) A
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 14
CONNECT IS E1 RC AT 15
DEFAULT MLEVEL IS ATOM
GGCAT IS UNS AT 12
DEFAULT ECLEVEL IS LIMITED
```

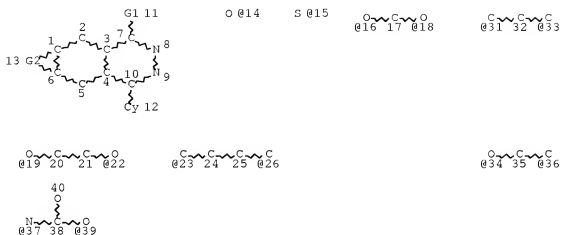
```
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
```

NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE

L10 56 SEA FILE=REGISTRY SSS FUL L8

L13 STR



VAR G1=14/15

VAR G2=16-6 18-1/19-6 22-1/31-6 33-1/23-6 26-1/34-6 36-1/36-6 34-1/37-6 3

9-1/39-6 37-1

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 14

CONNECT IS E1 RC AT 15

CONNECT IS E1 RC AT 40

DEFAULT MLEVEL IS ATOM

GGCAT IS UNS AT 12

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 36

STEREO ATTRIBUTES: NONE

L15 37 SEA FILE=REGISTRY SUB=L10 SSS FUL L13

100.0% PROCESSED 56 ITERATIONS

37 ANSWERS

SEARCH TIME: 00.00.01

=> d que nos l17

L8 STR

L10 56 SEA FILE=REGISTRY SSS FUL L8

L13 STR

L15 37 SEA FILE=REGISTRY SUB=L10 SSS FUL L13

L17 ANALYZE PLU=ON L15 1- LC : 8 TERMS

=> d l17 1-

L17 ANALYZE L15 1- LC : 8 TERMS

TERM # # OCC # DOC % DOC LC

```

-----
1      36      36  97.30  CA
2      36      36  97.30  CAPLUS
3      21      21  56.76  CASREACT
4      14      14  37.84  TOXCENTER
5       7       7  18.92  USPATFULL
6       1       1   2.70  BEILSTEIN
7       1       1   2.70  CAOLD
8       1       1   2.70  CHEMCATS
*****  END OF L17*****

```

=> d que nos 131

```

L1      1 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  US2004-772445/APPS
L8      STR
L10     56 SEA FILE=REGISTRY SSS FUL L8
L13     STR
L15     37 SEA FILE=REGISTRY SUB=L10 SSS FUL L13
L19     QUE SPE=ON  ABB=ON  PLU=ON  UPASANI, R?/AU
L20     QUE SPE=ON  ABB=ON  PLU=ON  CAI, S?/AU
L21     QUE SPE=ON  ABB=ON  PLU=ON  LAN, N?/AU
L22     QUE SPE=ON  ABB=ON  PLU=ON  WANG, Y?/AU
L23     QUE SPE=ON  ABB=ON  PLU=ON  FIELD, G?/AU
L24     QUE SPE=ON  ABB=ON  PLU=ON  FICK, D?/AU
L25     QUE SPE=ON  ABB=ON  PLU=ON  (COCENSYS OR (PURDUE(1W)PHAR
      MA) OR (EURO(1W)CELTIQUE))/CS,SO,PA
L27     17 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L15
L28     1 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L27 AND (L19 OR L20
      OR L21 OR L22 OR L23 OR L24 OR L25)
L29     1 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L1 AND L28
L30     1 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  (L28 OR L29)
L31     16 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L27 NOT L30

```

=> d his 134

```

      (FILE 'USPATFULL, USPATOLD, USPAT2, CASREACT, TOXCENTER' ENTERED AT
      15:31:58 ON 04 DEC 2008)
L34     6 S L32 NOT L33

```

=> d que nos 134

```

L8      STR
L10     56 SEA FILE=REGISTRY SSS FUL L8
L13     STR
L15     37 SEA FILE=REGISTRY SUB=L10 SSS FUL L13
L19     QUE SPE=ON  ABB=ON  PLU=ON  UPASANI, R?/AU
L20     QUE SPE=ON  ABB=ON  PLU=ON  CAI, S?/AU
L21     QUE SPE=ON  ABB=ON  PLU=ON  LAN, N?/AU
L22     QUE SPE=ON  ABB=ON  PLU=ON  WANG, Y?/AU
L23     QUE SPE=ON  ABB=ON  PLU=ON  FIELD, G?/AU
L24     QUE SPE=ON  ABB=ON  PLU=ON  FICK, D?/AU
L25     QUE SPE=ON  ABB=ON  PLU=ON  (COCENSYS OR (PURDUE(1W)PHAR
      MA) OR (EURO(1W)CELTIQUE))/CS,SO,PA
L32     9 SEA L15
L33     3 SEA L32 AND (L19 OR L20 OR L21 OR L22 OR L23 OR L24 OR L25)
L34     6 SEA L32 NOT L33

```

=> d que nos 135

```

L8      STR

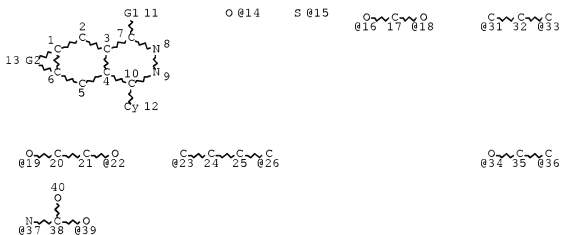
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L10 56 SEA FILE=REGISTRY SSS FUL L8
 L13 STR
 L15 37 SEA FILE=REGISTRY SUB=L10 SSS FUL L13
 L35 1 SEA FILE=CAOLD SPE=ON ABB=ON PLU=ON L15

=> d que nos 136
 L36 2 SEA FILE=HCAPLUS SPE=ON ABB=ON PLU=ON CA52:15486I/OREF

=> d que nos 137
 L8 STR
 L10 56 SEA FILE=REGISTRY SSS FUL L8
 L13 STR
 L15 37 SEA FILE=REGISTRY SUB=L10 SSS FUL L13
 L37 3 SEA FILE=CHEMCATS SPE=ON ABB=ON PLU=ON L15

=> d que stat 141
 L13 STR



VAR G1=14/15
 VAR G2=16-6 18-1/19-6 22-1/31-6 33-1/23-6 26-1/34-6 36-1/36-6 34-1/37-6 3
 9-1/39-6 37-1
 NODE ATTRIBUTES:
 CONNECT IS E1 RC AT 14
 CONNECT IS E1 RC AT 15
 CONNECT IS E1 RC AT 40
 DEFAULT MLEVEL IS ATOM
 GGCAT IS UNS AT 12
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 36

STEREO ATTRIBUTES: NONE
 L41 4 SEA FILE=CHEMINFORMRX SSS FUL L13 (8 REACTIONS)

100.0% DONE 1376 VERIFIED 8 HIT RXNS 4 DOCS
 SEARCH TIME: 00.00.22

=> d que nos l43

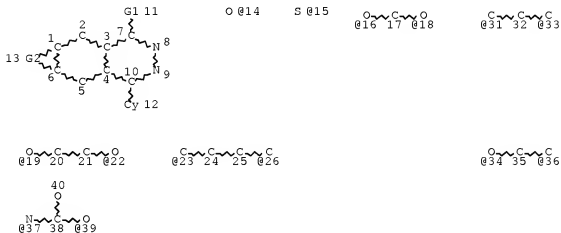
```

L13          STR
L19          QUE SPE=ON ABB=ON PLU=ON UPASANI, R?/AU
L20          QUE SPE=ON ABB=ON PLU=ON CAI, S?/AU
L21          QUE SPE=ON ABB=ON PLU=ON LAN, N?/AU
L22          QUE SPE=ON ABB=ON PLU=ON WANG, Y?/AU
L23          QUE SPE=ON ABB=ON PLU=ON FIELD, G?/AU
L24          QUE SPE=ON ABB=ON PLU=ON FICK, D?/AU
L25          QUE SPE=ON ABB=ON PLU=ON (COCENSYS OR (PURDUE(1W)PHAR
          MA) OR (EURO(1W)CELIQUE)) /CS,SO,PA
L41          4 SEA FILE=CHEMINFORMRX SSS FUL L13 (      8 REACTIONS)
L42          0 SEA FILE=CHEMINFORMRX SPE=ON ABB=ON PLU=ON L41 AND (L19 OR
          L20 OR L21 OR L22 OR L23 OR L24 OR L25)
L43          4 SEA FILE=CHEMINFORMRX SPE=ON ABB=ON PLU=ON L41 NOT L42

```

=> d que stat l45

L13 STR



VAR G1=14/15

VAR G2=16-6 18-1/19-6 22-1/31-6 33-1/23-6 26-1/34-6 36-1/36-6 34-1/37-6 3
9-1/39-6 37-1

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 14

CONNECT IS E1 RC AT 15

CONNECT IS E1 RC AT 40

DEFAULT MLEVEL IS ATOM

GGCAT IS UNS AT 12

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 36

STEREO ATTRIBUTES: NONE

L45 8 SEA FILE=WPIX SSS FUL L13

100.0% PROCESSED

599 ITERATIONS

8 ANSWERS

SEARCH TIME: 00.00.04

```
=> d que nos 151
L2      1 SEA FILE=WPIX SPE=ON  ABB=ON  PLU=ON  US2004-772445/APPS
L13     STR
L19     QUE SPE=ON  ABB=ON  PLU=ON  UPASANI, R?/AU
L20     QUE SPE=ON  ABB=ON  PLU=ON  CAI, S?/AU
L21     QUE SPE=ON  ABB=ON  PLU=ON  LAN, N?/AU
L22     QUE SPE=ON  ABB=ON  PLU=ON  WANG, Y?/AU
L23     QUE SPE=ON  ABB=ON  PLU=ON  FIELD, G?/AU
L24     QUE SPE=ON  ABB=ON  PLU=ON  FICK, D?/AU
L25     QUE SPE=ON  ABB=ON  PLU=ON  (COCENSYS OR (PURDUE(1W)PHAR
      MA) OR (EURO(1W)CELTIQUE))/CS,SO,PA
L45     8 SEA FILE=WPIX SSS FUL L13
L46     1 SEA FILE=WPIX SPE=ON  ABB=ON  PLU=ON  (RA00N1/DCN OR RA00N2/DCN
      OR RA00N3/DCN OR RA00N4/DCN OR RA00N5/DCN OR RA00N6/DCN OR
      RA00N7/DCN OR RA00N8/DCN) OR L45/DCR
L47     1 SEA FILE=WPIX SPE=ON  ABB=ON  PLU=ON  L46 AND (L19 OR L20 OR
      L21 OR L22 OR L23 OR L24 OR L25)
L49     1 SEA FILE=WPIX SPE=ON  ABB=ON  PLU=ON  L47 AND L2
L50     1 SEA FILE=WPIX SPE=ON  ABB=ON  PLU=ON  L47 OR L49
L51     0 SEA FILE=WPIX SPE=ON  ABB=ON  PLU=ON  L46 NOT L50
```

```
=> dup rem 131 134 135 136 137 143 151
```

L51 HAS NO ANSWERS

DUPLICATE IS NOT AVAILABLE IN 'CAOLD, CHEMCATS, CHEMINFORMRX'.

ANSWERS FROM THESE FILES WILL BE CONSIDERED UNIQUE

FILE 'HCAPLUS' ENTERED AT 15:45:19 ON 04 DEC 2008

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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FILE 'CASREACT' ENTERED AT 15:45:19 ON 04 DEC 2008

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FILE 'TOXCENTER' ENTERED AT 15:45:19 ON 04 DEC 2008

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FILE 'CHEMCATS' ENTERED AT 15:45:19 ON 04 DEC 2008

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FILE 'CHEMINFORMRX' ENTERED AT 15:45:19 ON 04 DEC 2008

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PROCESSING COMPLETED FOR L31

PROCESSING COMPLETED FOR L34

PROCESSING COMPLETED FOR L35

PROCESSING COMPLETED FOR L36

PROCESSING COMPLETED FOR L37

PROCESSING COMPLETED FOR L43

10/772,445

PROCESSING COMPLETED FOR L51

L55 24 DUP REM L31 L34 L35 L36 L37 L43 L51 (8 DUPLICATES REMOVED)
 ANSWERS '1-16' FROM FILE HCAPLUS
 ANSWER '17' FROM FILE CAOLD
 ANSWERS '18-20' FROM FILE CHEMCATS
 ANSWERS '21-24' FROM FILE CHEMINFORMRX

=> file stnguide

FILE 'STNGUIDE' ENTERED AT 15:45:37 ON 04 DEC 2008
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FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Nov 21, 2008 (20081121/UP).

=> d bib ed abs hitind hitstr 1-16
 YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS, CAOLD, CHEMCATS, CHEMINFORMRX' -
 CONTINUE? (Y)/N:y

L55 ANSWER 1 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 1

ACCESSION NUMBER: 2007:1295143 HCAPLUS Full-text

DOCUMENT NUMBER: 148:168645

TITLE: Iptycene-Derived Pyridazines and Phthalazines

AUTHOR(S): Bouffard, Jean; Eaton, Robert F.; Mueller, Peter;
 Swager, Timothy M.

CORPORATE SOURCE: Department of Chemistry, Massachusetts Institute of
 Technology, Cambridge, MA, 02139, USA

SOURCE: Journal of Organic Chemistry (2007), 72(26),
 10166-10180

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 148:168645

ED Entered STN: 15 Nov 2007

AB The synthesis of new heterocyclic oligo(phenylene) analogs based on soluble,
 non-aggregating 1,2-diazines is reported. Improved palladium-catalyzed
 reductive coupling methods were developed to allow for the preparation of
 large quantities of iptycene-derived bipyridazine compds. and biphthalazine
 compds., and the controlled synthesis of well-defined oligomers up to
 sexipyridazine. Crystallog., spectroscopic, and computational evidence
 indicate that in these analogs, hindrance at the ortho position is relaxed
 relative to poly(phenylenes). The resulting building blocks are promising for
 incorporation in conjugated electronics materials and as new iptycene-derived
 ligands for transition metals.

CC 28-15 (Heterocyclic Compounds (More Than One Hetero Atom))

IT 1625-81-6P 1625-82-7P 1625-83-8P,
 9,10-Dihydro-9,10(3',4')-furanoanthracene-12,14-dione 56306-24-2P
 56306-43-5P 123685-23-4P 272111-33-8P 937081-42-0P 937081-43-1P
 937081-49-7P 937081-50-0P 1001639-33-3P 1001639-35-5P
 1001639-36-6P 1001639-37-7P 1001639-38-8P 1001639-39-9P
 1001639-41-3P 1001639-43-5P 1001639-46-8P 1001639-47-9P
 1001639-50-4P 1001639-52-6P 1001639-55-9P 1001639-58-2P
 1001639-59-3P 1001639-61-7P 1001639-63-9P 1001639-64-0P
 1001639-66-2P 1001639-68-4P 1001639-71-9P 1001639-80-0P
 1001639-89-9P 1001639-93-5P 1001639-95-7P 1001640-05-6P
 1001640-06-7P 1001640-10-3P 1001640-24-9P

1001898-97-0P 1001898-99-1P 1001899-01-9P

1001899-70-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

(preparation of pyridazine and phthalazine derivs. of iptycenes,
 11[1',2']benzenonaphtho[2,3-d]pyridazine,
 6,11[1',2']benzenonaphtho[2,3-g]phthalazine derivs.)

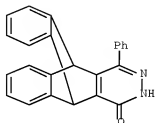
IT 1001639-89-9P 1001640-06-7P 1001640-10-3P

1001898-98-1P 1001899-01-9P

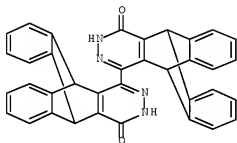
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

(preparation of pyridazine and phthalazine derivs. of iptycenes,
 11[1',2']benzenonaphtho[2,3-d]pyridazine,
 6,11[1',2']benzenonaphtho[2,3-g]phthalazine derivs.)

RN 1001639-89-9 HCAPLUS

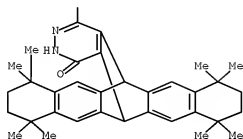
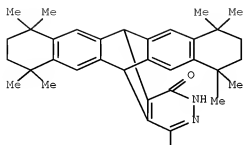
CN 5,10[1',2']-Benzenobenzo[g]phthalazin-1(2H)-one, 5,10-dihydro-4-phenyl-
(CA INDEX NAME)

RN 1001640-06-7 HCAPLUS

CN [1,1'-Bi-5,10[1',2']-benzenobenzo[g]phthalazine]-4,4'(3H,3'H)-dione,
5,5',10,10'-tetrahydro- (CA INDEX NAME)

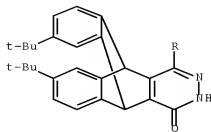
RN 1001640-10-3 HCAPLUS

CN [1,1'-Bi-5,12[2',3']-naphthalenonaphtho[2,3-g]phthalazine]-4,4'(3H,3'H)-
dione, 5,7,8,9,10,12,16,17,18,19-decahydro-7,7,10,10,16,16,19,19-
octamethyl- (CA INDEX NAME)

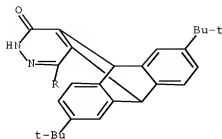


RN 1001898-98-1 HCAPLUS

CN [1,1'-Bi-5,10[1',2']-benzenobenzo[g]phthalazine]-4,4'-(3H,3'H)-dione,
7,7',15,15'-tetrakis(1,1-dimethylethyl)-5,5',10,10'-tetrahydro-,
stereoisomer (CA INDEX NAME)



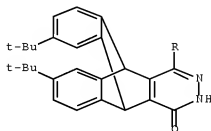
PAGE 2-A



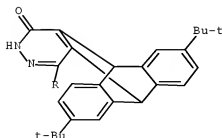
RN 1001899-01-9 HCAPLUS

CN [1,1'-Bi-5,10[1',2']-benzenobenzo[g]phthalazine]-4,4' (3H,3'H)-dione,
7,7',15,15'-tetrakis(1,1-dimethylethyl)-5,5',10,10'-tetrahydro-,
stereoisomer (CA INDEX NAME)

PAGE 1-A



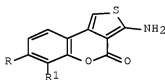
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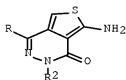
REFERENCE COUNT:

113 THERE ARE 113 CITED REFERENCES AVAILABLE FOR
THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L55 ANSWER 2 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 2
 ACCESSION NUMBER: 2005:342380 HCAPLUS [Full-text](#)
 DOCUMENT NUMBER: 144:88229
 TITLE: Studies with condensed thiophenes: Reactivity of condensed aminothiophenes toward carbon and nitrogen electrophiles
 AUTHOR(S): Al-Saleh, Balkis; Abdelkhalik, Mervat M.; El-Asasery, Morsy A.; Elnagdi, Mohamed H.
 CORPORATE SOURCE: Department of Chemistry, Faculty of Science, University of Kuwait, Safat, 13060, Kuwait
 SOURCE: Journal of Chemical Research (2005), (1), 23-26
 CODEN: JCROA4
 PUBLISHER: Science Reviews
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 144:88229
 ED Entered STN: 21 Apr 2005
 GI



I



II

AB The condensed aminothiophenes I (R, R1 = H; RR1 = C4H4) and II (R = CO2Et, R2 = Ph; R = benzotriazol-1-yl, R2 = 4-MeC6H4) react with 1,4-naphthoquinone in refluxing ethanol to yield products of addition followed by hydrogen sulfide elimination in a Diels-Alder-type reaction. When the reaction is carried out under microwave irradiation a dipolar addition occurred affording products of substitution at C(1). Compds. I and II coupled with aromatic diazonium salts to yield arylazo derivs. where coupling occurred at C(1). Reaction of I and II with DMF dimethylacetal yielded amidines.

CC 28-15 (Heterocyclic Compounds (More Than One Hetero Atom))

IT

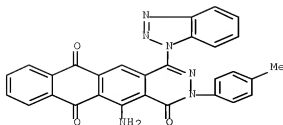
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| 872425-23-5P | 872425-24-6P | 872425-25-7P | 872425-26-8P | |
| 872425-27-9P | 872425-28-0P | 872425-29-1P | 872425-30-4P | 872425-31-5P |
| 872425-32-6P | 872425-33-7P | 872425-34-8P | 872425-35-9P | 872425-36-0P |
| 872425-39-3P | 872425-40-6P | 872425-41-7P | 872425-42-8P | |

RL: SPN (Synthetic preparation); PREP (Preparation)
 (reactions of condensed aminothiophenes with carbon and nitrogen electrophiles)

IT ~~872425-25-7P~~
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (reactions of condensed aminothiophenes with carbon and nitrogen electrophiles)

RN 872425-25-7 HCAPLUS

CN Naphtho[2,3-g]phthalazine-1,6,11(2H)-trione,
 12-amino-4-(1H-benzotriazol-1-yl)-2-(4-methylphenyl)- (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L55 ANSWER 3 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 3

ACCESSION NUMBER: 2002:224723 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 137:194982

TITLE: Triazolo- and imidazophthalazines, are they non-competitive AMPA antagonists?

AUTHOR(S): Solyom, Sandor; Hamori, Tamas; Borosy, Andras P.; Tarnawa, Istvan; Berzsényi, Pal; Pallagi, Istvan

CORPORATE SOURCE: IVAX Drug Research Institute, Ltd, Budapest, H-1045, Hung.

SOURCE: Medicinal Chemistry Research (2002), 11(1), 39-49

CODEN: MCREEB; ISSN: 1054-2523

PUBLISHER: Birkhaeuser Boston

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:194982

ED Entered STN: 25 Mar 2002

AB Earlier structure-activity relationship studies within the 2,3-benzodiazepine family had revealed that the 3-acyl-4-Me part of 2, an active non-competitive AMPA antagonist, can be substituted by condensed azolenings at the same position preserving or improving biol. activity. This suggests that the same structural features can be applied to some phthalazine derivs. that have been shown to possess non-competitive AMPA antagonist activity. Therefore new [1,2,4]triazolo[3,4-a]- and imidazo[2,1-a]phthalazines of type 21 were synthesized applying known and new methods in multistep routes. The resulted compds. had no pharmacol. activity either in vitro (up to 20 μ M) or in vivo (up to 100 mg/kg i.p., or 200 mg/kg orally). To find a possible explanation for the lack of AMPA antagonistic potencies a computer aided mol. modeling study was performed.

CC 1-3 (Pharmacology)

Section cross-reference(s): 27

| | | | | | | |
|----|------------------------------|--------------|--------------|--------------|--------------|--|
| IT | 295793-38-3P | 452973-84-1P | 452973-85-2P | 452973-86-3P | | |
| | 452973-87-4P | 452973-88-5P | 452973-89-6P | 452973-90-9P | 452973-91-0P | |
| | 452973-92-1P | 452973-93-2P | 452973-94-3P | 452973-95-4P | 452973-96-5P | |
| | 452973-97-6P | 452973-98-7P | 452973-99-8P | 452974-00-4P | 452974-01-5P | |
| | 452974-02-6P | 452974-03-7P | 452974-04-8P | 452974-05-9P | 452974-06-0P | |
| | 452974-07-1P | 452974-08-2P | 452974-09-3P | 452974-10-6P | 452974-11-7P | |
| | 452974-12-8P | 452974-13-9P | | | | |

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(triazolo- and imidazophthalazines, are they non-competitive AMPA antagonists)

IT [295793-38-3P](#)

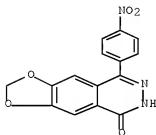
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(triazolo- and imidazophthalazines, are they non-competitive AMPA antagonists)

RN 295793-38-3 HCAPLUS

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(4-nitrophenyl)- (CA INDEX NAME)



REFERENCE COUNT: 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L55 ANSWER 4 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 4

ACCESSION NUMBER: 2000:457925 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 133:246792

TITLE: Synthesis and anticonvulsant activity of novel and

potent 6,7-methylenedioxypthalazin-1(2H)-ones
Grasso, Silvana; De rro, Giovambattista; De Sarro,
Angela; Micale, Nicola; Zappala, Maria; Puja, Giulia;
Baraldi, Mario; De icheli, Carlo

CORPORATE SOURCE: Dipartimento Farmaco-Chimico and Istituto di
Farmacologia, Universita di Messina, Messina, Italy

SOURCE: Journal of Medicinal Chemistry (2000), 43(15),
2851-2859

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

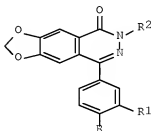
DOCUMENT TYPE: Journal

LANGUAGE: English

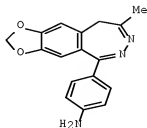
OTHER SOURCE(S): CASREACT 133:246792

ED Entered STN: 09 Jul 2000

GI

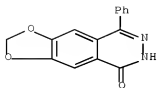


I



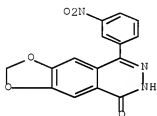
II

- AB In this paper, the authors describe the synthesis of a series of novel substituted 4-aryl-6,7-methylenedioxyphthalazin-1(2H)-ones I (R = H, O2N, H2N; R1 = H, O2N, H2N; R2 = H, R3NHCO; R3 = Me, Et, EtCH2, Bu, BuCH2, cyclohexyl). The anticonvulsant activity of these compds. against audiogenic seizures was evaluated in DBA/2 mice after i.p. (i.p.) injection. Most of these derivs. are more active than 1-(4-aminophenyl)-4-methyl-7,8-methylenedioxy-5H-2,3-benzodiazepine II (GYKI 52466), a well-known noncompetitive AMPA receptor antagonist. As deduced by the rotarod test, all the compds. exhibit a toxicity lower than that of II. Within the series of derivs. submitted to investigation, 4-(4-aminophenyl)-2-butylcarbamoyl-6,7-methylenedioxyphthalazin-1(2H)-one I (R = H2N; R1 = H; R2 = BuNHCO) proved to be the most active compound and is 11-fold more potent than II [i.e., ED50 3.25 μ mol/kg for I (R = H2N; R1 = H; R2 = BuNHCO) vs. ED50 35.8 μ mol/kg for II]. When compared to II, compound I (R = H2N; R1 = H; R2 = BuNHCO) as well as its analog 4-(4-aminophenyl)-6,7-methylenedioxyphthalazin-1(2H)-one I (R = H2N; R1 = R2 = H) show a longer lasting anticonvulsant activity. Compound I (R = H2N; R1 = H; R2 = BuNHCO) also effectively suppresses seizures induced in Swiss mice by maximal electroshock (MES) and pentylenetetrazole (PTZ). Furthermore, it antagonizes in vivo seizures induced by 2-amino-3-(3-hydroxy-5-methylisoxazol-4-yl)propionic acid (AMPA), 2-amino-3-(3-hydroxy-5-tert-butylisoxazol-4-yl)propionic acid (ATPA), and kainate (KA), and its anticonvulsant activity is reversed by pretreatment with aniracetam. Using the patch-clamp technique, the capability of derivs. III and IV to antagonize KA-evoked currents in primary cultures of granule neurons was tested. They behaved as antagonists, but they proved to be less effective than II and 1-(4-aminophenyl)-3,4-dihydro-4-methyl-3- N-methylcarbamoyl-7,8-methylene dioxy-5H-2,3-benzodiazepine (GYKI 53655) to reduce the KA-evoked currents.
- CC 1-3 (Pharmacology)
- IT 295793-36-1P 295793-37-2P 295793-38-3P
295793-40-7P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and anticonvulsant activity of (methylenedioxy)phthalazinones)
- IT 295793-39-4P 295793-41-8P 295793-42-9P
295793-43-6P 295793-44-1P 295793-45-2P
295793-46-3P 295793-47-4P 295793-48-5P
295793-49-6P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (preparation and anticonvulsant activity of (methylenedioxy)phthalazinones)
- IT 295793-36-1P 295793-37-2P 295793-38-3P
295793-40-7P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and anticonvulsant activity of (methylenedioxy)phthalazinones)
- RN 295793-36-1 HCAPLUS
- CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-phenyl- (CA INDEX NAME)



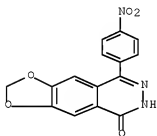
RN 295793-37-2 HCAPLUS

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(3-nitrophenyl)- (CA INDEX NAME)



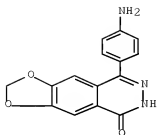
RN 295793-38-3 HCAPLUS

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(4-nitrophenyl)- (CA INDEX NAME)



RN 295793-40-7 HCAPLUS

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(4-aminophenyl)- (CA INDEX NAME)



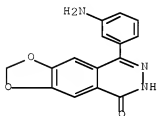
IT 295793-39-4P 295793-41-8P 295793-42-9P
295793-43-8P 295793-44-1P 295793-45-2P
295793-46-3P 295793-47-4P 295793-48-5P
295793-49-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and anticonvulsant activity of (methylenedioxy)phthalazinones)

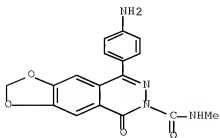
RN 295793-39-4 HCAPLUS

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(3-aminophenyl)- (CA INDEX NAME)



RN 295793-41-8 HCAPLUS

CN 1,3-Dioxolo[4,5-g]phthalazine-6(5H)-carboxamide,
 8-(4-aminophenyl)-N-methyl-5-oxo- (CA INDEX NAME)

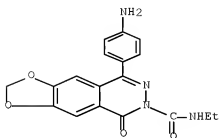


RN 295793-42-9 HCAPLUS

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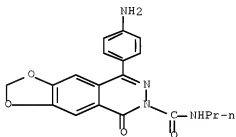
10/772,445

8-(4-aminophenyl)-N-ethyl-5-oxo- (CA INDEX NAME)



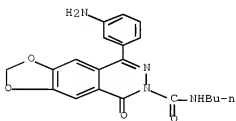
RN 295793-43-0 HCAPLUS

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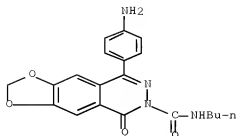
RN 295793-44-1 HCAPLUS

CN 1,3-Dioxolo[4,5-g]phthalazine-6(5H)-carboxamide,
8-(3-aminophenyl)-N-butyl-5-oxo- (CA INDEX NAME)



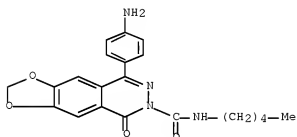
RN 295793-45-2 HCAPLUS

CN 1,3-Dioxolo[4,5-g]phthalazine-6(5H)-carboxamide,
8-(4-aminophenyl)-N-butyl-5-oxo- (CA INDEX NAME)



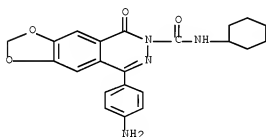
RN 295793-46-3 HCAPLUS

CN 1,3-Dioxolo[4,5-g]phthalazine-6(5H)-carboxamide,
8-(4-aminophenyl)-5-oxo-N-pentyl- (CA INDEX NAME)



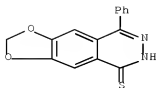
RN 295793-47-4 HCAPLUS

CN 1,3-Dioxolo[4,5-g]phthalazine-6(5H)-carboxamide,
8-(4-aminophenyl)-N-cyclohexyl-5-oxo- (CA INDEX NAME)

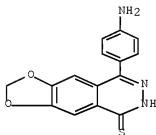


RN 295793-48-5 HCAPLUS

CN 1,3-Dioxolo[4,5-g]phthalazine-5(6H)-thione, 8-phenyl- (CA INDEX NAME)

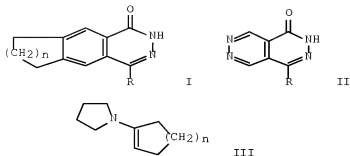


RN 295793-49-6 HCAPLUS
 CN 1,3-Dioxolo[4,5-g]phthalazine-5(6H)-thione, 8-(4-aminophenyl)- (CA INDEX NAME)



REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L55 ANSWER 5 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 5
 ACCESSION NUMBER: 1995:956557 HCAPLUS [Full-text](#)
 DOCUMENT NUMBER: 124:146037
 ORIGINAL REFERENCE NO.: 124:27161a,27164a
 TITLE: Inverse-electron-demand Diels-Alder reactions of condensed pyridazines. 8. Convenient synthesis of cycloalkene-fused phthalazinones
 AUTHOR(S): Haider, Norbert
 CORPORATE SOURCE: Inst. Pharmaceutical Chem., Univ. Vienna, Vienna, A-1090, Austria
 SOURCE: Heterocycles (1995), 41(11), 2519-25
 CODEN: HTCYAM; ISSN: 0385-5414
 PUBLISHER: Japan Institute of Heterocyclic Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 124:146037
 ED Entered STN: 01 Dec 1995
 GI



AB A series of cycloalkene-annulated phthalazin-1(2H)-ones I (R = Et, Ph, n = 1-4) was prepared in high yields by a one-pot procedure, employing pyridazino[4,5-d]pyridazin-1(2H)-ones II as azadienes and cyclic enamines III as dienophiles in an inverse-electron-demand Diels-Alder reaction, followed by acid-catalyzed aromatization.

CC 28-15 (Heterocyclic Compounds (More Than One Hetero Atom))

IT 173463-56-4P 173463-57-5P 173463-58-6P 173463-59-7P
173463-60-0P 173463-61-1P 173463-62-2P 173463-63-3P 173463-64-4P
173463-65-5P 173463-66-6P 173463-67-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of cycloalkene-fused phthalazinones by Diels-Alder of condensed pyridazines with cyclic enamines)

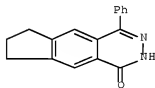
IT 173463-57-5P 173463-59-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of cycloalkene-fused phthalazinones by Diels-Alder of condensed pyridazines with cyclic enamines)

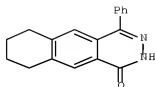
RN 173463-57-5 HCAPLUS

CN 1H-Cyclopenta[g]phthalazin-1-one, 2,6,7,8-tetrahydro-4-phenyl- (CA INDEX NAME)



RN 173463-59-7 HCAPLUS

CN Benzo[g]phthalazin-1(2H)-one, 6,7,8,9-tetrahydro-4-phenyl- (CA INDEX NAME)



L55 ANSWER 6 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 6

ACCESSION NUMBER: 1958:87985 HCAPLUS Full-text

DOCUMENT NUMBER: 52:87985

ORIGINAL REFERENCE NO.: 52:15485g-1,15486a-1

TITLE: Selective reduction by calcium hexammine. I. Aromatic hydrocarbons

AUTHOR(S): Boer, H.; Duinker, P. M.

CORPORATE SOURCE: Roy. Shell Lab., Amsterdam

SOURCE: Recueil des Travaux Chimiques des Pays-Bas et de la Belgique (1958), 77, 346-59

CODEN: RTCPB4; ISSN: 0370-7539

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 52:87985

ED Entered STN: 22 Apr 2001

AB Under carefully adjusted reaction conditions polynuclear aromatic hydrocarbons were selectively reduced by $\text{Ca}(\text{NH}_3)_6$ (I) to compds. containing only one isolated benzene ring. The hydrocarbons used were purified com. or synthetic samples and the details of synthesis and phys. properties are tabulated. Carefully dried liquid NH_3 and a known weight of Ca chips siphoned under N into an Et2O solution of hydrocarbon (30 millimoles/100 ml. Et2O), the mixture stirred vigorously with evaporation of the NH_3 , kept 23 hrs., filtered (N atm) without suction, and the filtrate evaporated gave a clear residue of product. Ca powder in Et2O at 0° saturated with a slight excess of NH_3 , the hydrocarbon added carefully (4 moles NH_3 liberated by 1 mole reactive I), and the mixture worked up as above gave the reduced product. Ca was calculated on the basis of conversion of polyaromatics to monoaromatics with 50% excess and recoveries were generally better than 95%. Details of general methods for determining the reaction products by catalytic hydrogenation, percolation, ultraviolet spectroscopy, gas-liquid chromatography, ozonometry, and refractive index detns. are given. Comparison of the ultraviolet spectra before and after catalytic hydrogenation showed conjugated cyclohexadienes to be absent in the reaction products of alkylbenzenes on reduction by the "liquid ammonia" method. In a few expts. the product was percolated over silica and the absence of alkylcyclohexanes demonstrated. From the total unsatn., determined ozonometrically, and the amount of unreacted aromatics, as found by ultraviolet spectral analysis after hydrogenation, the contents of alkylcyclohexene and alkylcyclohexadiene were calculated and the data obtained confirmed by refractive index analyses. Results of the "liquid ammonia" reduction of alkylbenzenes are tabulated (hydrocarbon, weight-% unreacted, weight-% cyclohexadienes, and weight-% cyclohexenes given): C_6H_6 , -, -, 100; PhMe, 10, 32, 58; PhEt, 19, 21, 60; o-xylene, 68, 17, 15; m-xylene, 30, 35, 35; p-xylene, 42, 40, 18. Reduction of 1,2,4- and 1,3,5- $\text{C}_6\text{H}_3\text{Me}_3$, 1,2,4,5- $\text{C}_6\text{H}_2\text{Me}_4$, and C_6Me_6 gave 86, 72, 94, and 100% unreacted material and 14, 28, 6, and 0% unidentified mixts. of cyclohexadienes and cyclohexenes. A number of compds. containing more than one aromatic ring were treated with I by the same procedure (polynuclear aromatic, weight-% monoaromatics, and weight-% nonaromatic cycloalkenes given): Ph2, 55, 45; Ph2CH2, 56, 44; ClO8H, 40, 60;

anthracene, -, 100; phenanthrene, 42, 58; 1-methyl-7-isopropylphenanthrene, 85, 15; triphenylene, 63, 37. Thus, the polynuclear aromatics are quantitatively reduced to benzene derivs. which may undergo partial reduction to cycloalkenes. In a series of reductions of 1,2,3,4-tetrahydronaphthalene by the "gaseous ammonia" method it was shown that the C6H6 nucleus was but very little attacked at 0° in 1 hr. The results of reduction of various polynuclear aromatics under these conditions are summarized [aromatic, weight-% unreacted, weight-% benzene derivs. (composition of monoaromatic fraction) and weight-% nonaromatic cycloalkenes given]: Ph2, 0.4, 99 (21% phenylcyclohexene and 79% phenylcyclohexane), -; Ph2CH2, 84, 16 (phenylcyclohexenylmethane and phenylcyclohexadienylmethane), -; (PhCH2)2, 95, 5 (PhCH2CH2C6H9), -; C10H8, -, 94 (1,2,3,4-tetrahydronaphthalene), 6 (mainly C10H16); acenaphthene, trace, 100 (tetrahydroacenaphthene), -; 2,3,6-Me3C10H5, 1, 99 (8% trimethyltetrahydronaphthalene, 92% 1,4-dihydrotrimethylnaphthalene), -; anthracene, 0.17, - (9,10-dihydro- and hexahydroanthracene), -; phenanthrene, trace, 100 (7% hexahydrophenanthracene), -; phenanthrene, trace, 100 (7% hexa- and 93% octahydrophenanthrene), -. To demonstrate that alkenylbenzenes with a side-chain containing a double bond in conjunction with the aromatic nucleus are readily reduced with I, comparative reductions with Tetralin were made (compound, weight-% unreacted, weight-% indan, weight-% PhEt, and weight-% nonaromatic cycloalkenes given): indene, 30, 54, -, 15.5; styrene, -, -, 94, 2; indan, 90, 90, -, 8; Tetralin, 95, -, -, 5. It would appear that the reduction of indene to a nonaromatic cycloalkene takes place via an intermediate other than indan. The selectivity of I reduction made possible the preparation of compds. previously difficult to synthesize. Ground Ca (80 g.) in 1 l. dry Et2O at 0° saturated with a stream of dry NH3 (60 l./hr.) and diluted with 156 g. dry C6H6, the cooling bath removed, the NH3 evaporated 1.5 hrs., the residue acidified at -20°, and the washed and dried Et2O layer evaporated gave 142 g. product, n25D 1.4721 (containing 0.945 alkene-type double bond/mol.), converted to the tetrabromide and washed with hot MeOH; the mixture of 2 stereoisomeric tetrabromides, m. 176-81°, decomposed according to Huckel and Worffel (C.A. 50, 7093e) yielded 30% pure 1,4-cyclohexadiene, b774 88.7-9.1°, n20D 1.4722. Dry NH3 gas (30 l./hr.) passed 4 hrs. into 1 l. dry ether stirred with 60 g. powdered Ca and 60 g. phenanthrene, the mixture suction-filtered, the filter cake added portionwise to H2O, and the acidified solution extracted with Et2O gave 185 g. (3 consecutive preps.) containing 9% alkene compds. The material hydrogenated at 100°/200 atmospheric with Cu chromite catalyst, and the product percolated over silica and Al2O3 gave 176 g. octahydrophenanthrenes, n25D 1.5575, distilled over a 20-theoretical plate Vigreux column to show the presence of 45% sym. and 55% unsym. isomers, n25D 1.5461 and 1.5513, resp. Mixts. of alkyl-substituted Tetralins (II) were obtained from the alkylnaphthalenes by the "gaseous ammonia" technique and worked up as above; α - and β -methylnaphthalenes gave only II whereas the reaction product of 2,3-C10H6Me2 contained 14% aliphatic double bonds. Some remarks are made on the mechanism of the reaction.

CC 10 (Organic Chemistry)

IT 12133-31-2 29811-05-0 76044-99-0 101723-54-0 101789-59-7

~~109892-05-9~~ 114722-26-8

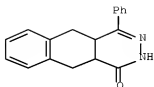
(Derived from data in the 6th Collective Formula Index (1957-1961))

IT ~~109892-05-9~~

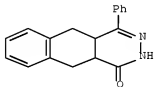
(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 109892-05-9 HCAPLUS

CN Benzo[g]phthalazin-1(2H)-one, 4a,5,10,10a-tetrahydro-4-phenyl- (CA INDEX NAME)



L55 ANSWER 7 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 7
 ACCESSION NUMBER: 1958:87986 HCAPLUS Full-text
 DOCUMENT NUMBER: 52:87986
 ORIGINAL REFERENCE NO.: 52:154861,15487a
 TITLE: Unsaturated hydrocarbons. III. New method of synthesis of aromatic hydrocarbons with a desired structure
 AUTHOR(S): Kotlyarevskii, I. L.; Zanina, A. S.; Lipovich, V. G.
 SOURCE: Zhurnal Prikladnoi Khimii (Sankt-Peterburg, Russian Federation) (1957), 30, 335-7
 CODEN: ZPKHAB; ISSN: 0044-4618
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 ED Entered STN: 22 Apr 2001
 AB See C.A. 51, 13790i.
 CC 10 (Organic Chemistry)
 IT 1559-81-5 1680-51-9 2809-64-5 3877-19-8 29811-05-0 76044-99-0
 101723-54-0 101789-59-7 109892-05-9 114722-26-8
 (Derived from data in the 6th Collective Formula Index (1957-1961))
 IT 109892-05-9
 (Derived from data in the 6th Collective Formula Index (1957-1961))
 RN 109892-05-9 HCAPLUS
 CN Benzo[g]phthalazin-1(2H)-one, 4a,5,10,10a-tetrahydro-4-phenyl- (CA INDEX NAME)



L55 ANSWER 8 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2005:430641 HCAPLUS Full-text
 DOCUMENT NUMBER: 143:165974
 TITLE: QSAR study of 2,3-benzodiazepin-4(thi)one- and 1,2-phthalazine-related negative allosteric modulators of the AMPA receptor: A structural descriptors-based reassessment
 AUTHOR(S): Buchwald, Peter; Einstein, Brandon; Bodor, Nicholas
 CORPORATE SOURCE: IVAX Research, Inc., Miami, FL, USA
 SOURCE: QSAR & Combinatorial Science (2005), 24(3), 325-331
 CODEN: QCSSAU; ISSN: 1611-020X
 PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal
 LANGUAGE: English
 ED Entered STN: 20 May 2005

AB In an attempt to establish statistically more rigorous and chemical more meaningful quant. structure-activity relationship (QSAR) equations, a reassessment of a recent study of in vivo anticonvulsant activity for a set of 2,3-benzodiazepin-4(thi)one- and 1,2-phthalazine-related allosteric AMPA antagonists (n=61) is presented. Contrary to the original, relatively nonspecific descriptor set, which included, for example, a number of topol. descriptors, specific structural descriptors that are much easier to interpret from a medicinal chemical point of view are used in this multiple linear regression-based approach. Only statistically significant descriptors have been retained in the final equation, and whereas they give about the same correlation as those of the original paper on the training set (r^2 of 0.79 vs. 0.76, $n=49$), they perform much better on the test set (predictive r^2 of 0.73 vs. 0.05; r^2 of 0.78 vs. 0.08, $n=12$). Descriptors found to be relevant are clearly related to substitutions at known pharmacophore positions, such as those corresponding to the 2,3-, 7,8- and 4'-positions of the benzodiazepine skeleton. Therefore, by a more careful selection of the descriptor set, both an improved prediction and a more intuitive quant. interpretation could be achieved for this set of allosteric AMPA antagonists.

CC 1-3 (Pharmacology)

IT 35011-63-3 41148-41-8 41148-42-9 47281-61-8 55507-15-8
 96315-84-3 96315-85-4 102693-05-0 102693-13-0 102693-14-1
 102693-24-3 173284-36-1 178616-26-7 187940-09-6 187940-20-1
 187940-28-9 187940-29-0 187940-30-3 187940-31-4 187940-33-6
 197368-44-8 197368-47-1 197368-49-3 197368-51-7 197368-92-6
 197369-07-6 213385-71-8 213385-72-9 213385-73-0 213385-74-1
 213385-76-3 213385-77-4 213385-78-5 213385-79-6 213385-80-9
 213385-81-0 231623-78-2 236109-55-0 236109-57-2 236109-58-3
 250699-34-4 250699-41-3 292858-36-7 292858-38-9 292858-39-0
 292858-40-3 292858-42-5 292858-46-9 295793-36-1
295793-39-4 295793-40-7 295793-41-8
295793-43-0 320349-99-3 320350-01-4 320350-02-5
 320350-03-6 320350-04-7 320350-05-8 320350-06-9 681457-29-4

RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(OSAR study of 2,3-benzodiazepin-4(thi)one- and 1,2-phthalazine-related neg. allosteric modulators of AMPA receptor and a structural descriptors-based reassessment)

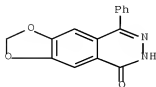
IT 295793-36-1 295793-39-4 295793-40-7
295793-41-8 295793-43-0

RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(OSAR study of 2,3-benzodiazepin-4(thi)one- and 1,2-phthalazine-related neg. allosteric modulators of AMPA receptor and a structural descriptors-based reassessment)

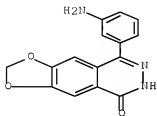
RN 295793-36-1 HCAPLUS

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-phenyl- (CA INDEX NAME)



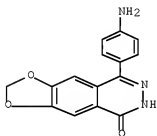
RN 295793-39-4 HCAPLUS

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(3-aminophenyl)- (CA INDEX NAME)



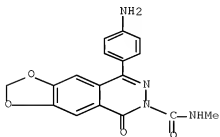
RN 295793-40-7 HCAPLUS

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(4-aminophenyl)- (CA INDEX NAME)



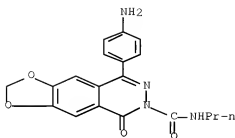
RN 295793-41-8 HCAPLUS

CN 1,3-Dioxolo[4,5-g]phthalazine-6(5H)-carboxamide, 8-(4-aminophenyl)-N-methyl-5-oxo- (CA INDEX NAME)



RN 295793-43-0 HCAPLUS

CN 1,3-Dioxolo[4,5-g]phthalazine-6(5H)-carboxamide, 8-(4-aminophenyl)-5-oxo-N-propyl- (CA INDEX NAME)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L55 ANSWER 9 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:168622 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 140:350044

TITLE: QSAR Study of Anticonvulsant Negative Allosteric Modulators of the AMPA Receptor

AUTHOR(S): Macchiarulo, Antonio; De Luca, Laura; Costantino, Gabriele; Barreca, Maria Letizia; Gitto, Rosaria; Pellicciari, Roberto; Chimirri, Alba

CORPORATE SOURCE: Dipartimento di Chimica e Tecnologia del Farmaco, Università di Perugia, Perugia, 06123, Italy

SOURCE: Journal of Medicinal Chemistry (2004), 47(7), 1860-1863

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 02 Mar 2004

AB A quant. structure-activity relation (QSAR) study was performed on a set of 49 neg. allosteric modulators of AMPA receptor, acting as anticonvulsant agents, using multiple linear regression. The predictive ability of the resulting model was evaluated against a set of 12 compds.; the results showed good statistics in regression and revealed high correlation between anticonvulsant activity and some electrotopol. descriptors.

CC 1-3 (Pharmacology)

IT 41148-41-8 41148-42-9 47281-61-8 55507-15-8 96315-84-3
 96315-85-4 102693-05-0 102693-13-0 102693-14-1 102693-24-3
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295793-39-4 295793-40-7 295793-41-8

295793-43-0

320349-99-3 320350-01-4 320350-02-5 681457-29-4

320350-03-6

320350-04-7

320350-05-8

320350-06-9

RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (QSAR of anticonvulsant neg. allosteric modulators of AMPA receptor)

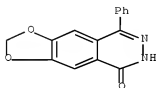
IT 295793-36-1 295793-39-4 295793-40-7

295793-41-8 295793-43-6

RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (QSAR of anticonvulsant neg. allosteric modulators of AMPA receptor)

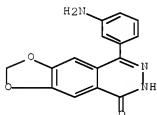
RN 295793-36-1 HCAPLUS

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-phenyl- (CA INDEX NAME)



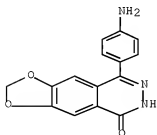
RN 295793-39-4 HCAPLUS

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(3-aminophenyl)- (CA INDEX NAME)



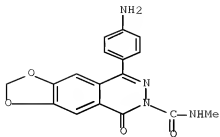
RN 295793-40-7 HCAPLUS

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(4-aminophenyl)- (CA INDEX NAME)

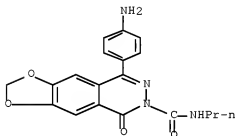


RN 295793-41-8 HCAPLUS

CN 1,3-Dioxolo[4,5-g]phthalazine-6(5H)-carboxamide, 8-(4-aminophenyl)-N-methyl-5-oxo- (CA INDEX NAME)



RN 295793-43-0 HCAPLUS
 CN 1,3-Dioxolo[4,5-g]phthalazine-6(5H)-carboxamide,
 8-(4-aminophenyl)-5-oxo-N-propyl- (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L55 ANSWER 10 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2004:205961 HCAPLUS Full-text
 DOCUMENT NUMBER: 142:197900
 TITLE: Product class 10: phthalazines
 AUTHOR(S): Haider, N.; Holzer, W.
 CORPORATE SOURCE: Germany
 SOURCE: Science of Synthesis (2004), 16, 315-372
 CODEN: SSCYJ9
 PUBLISHER: Georg Thieme Verlag
 DOCUMENT TYPE: Journal; General Review
 LANGUAGE: English

ED Entered STN: 15 Mar 2004

AB A review. Preparation is given for phthalazines via ring closure or transformation reactions, aromatization or substituent modification.

CC 28-0 (Heterocyclic Compounds (More Than One Hetero Atom))

| | | | | | |
|----|-------------|-------------|-------------|-------------|-------------|
| IT | 66645-92-9 | 66859-13-0 | 67081-02-1 | 70097-45-9 | 70801-31-9 |
| | 70801-33-1 | 73661-77-5 | 73661-78-6 | 73661-79-7 | 75998-18-4 |
| | 76240-43-2 | 76972-35-5 | 79690-84-9 | 84641-77-0 | 86355-12-6 |
| | 87255-76-3 | 89516-24-5 | 90719-21-4 | 90915-39-2 | 91054-33-0 |
| | 91566-88-0 | 92722-88-8 | 95884-14-3 | 97694-85-4 | 99161-49-6 |
| | 100448-45-1 | 100448-46-2 | 100537-30-2 | 101440-97-5 | 101889-52-5 |
| | 105850-89-3 | 112633-87-1 | 112633-89-3 | 114202-92-5 | 119838-09-4 |
| | 121561-18-0 | 122665-83-2 | 124433-93-8 | 129221-76-7 | 132960-21-5 |
| | 137207-61-5 | 137207-65-9 | 137382-32-2 | 137382-37-7 | 143915-58-6 |
| | 153078-00-3 | 153078-01-4 | 155937-09-0 | 155937-30-7 | 161851-52-1 |

| | | | | |
|-------------|-------------|-------------|-------------|------------------------|
| 170373-53-2 | 178309-37-0 | 183968-10-7 | 189213-58-9 | 210166-63-5 |
| 210166-73-7 | 219966-12-8 | 219966-14-0 | 226995-83-1 | 295793-36-1 |
| 297132-06-0 | 297132-07-1 | 297132-08-2 | 311339-02-3 | 350690-07-2 |
| 412339-50-5 | 479058-74-7 | 537033-42-4 | | |

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of phthalazines)

| | | | |
|----|--------------------------------|--------------------------------|--------------|
| IT | 119-39-1P, 1(2H)-Phthalazinone | 253-52-1P, Phthalazine | 484-23-1P |
| | 1445-69-8P | 2257-69-4P | 4673-39-6P |
| | 5004-46-6P | 5004-48-8P | 5784-45-2P |
| | 10132-01-1P | 13925-27-4P | 14503-64-1P |
| | 1(2H)-Phthalazinethione | 17341-79-6P | 17987-70-1P, |
| | 1,4-Phthalazinediamine | 19064-69-8P, 1-Phthalazinamine | 21131-44-2P |
| | 21452-56-2P | 21948-74-3P | 25947-13-1P |
| | 39794-30-4P | 40125-48-2P | 40848-53-1P |
| | 57835-96-8P | 63536-21-0P | 68775-89-3P |
| | 77533-21-2P | 81731-69-3P | 89891-73-6P |
| | 91587-99-4P | 94309-83-8P | 100881-26-3P |
| | 103286-04-0P | 105936-84-3P | 107558-48-5P |
| | 154822-28-3P | 154822-30-7P | 154822-32-9P |
| | 167705-73-9P | 173463-59-7P | 203929-42-4P |
| | 203929-44-6P | 203929-45-7P | 203929-47-9P |
| | 203929-53-7P | 203929-55-9P | 203929-56-0P |
| | 203929-63-9P | 203929-65-1P | 203929-66-2P |
| | 221632-73-1P | 221632-74-2P | 221632-75-3P |
| | | | 203929-49-1P |
| | | | 203929-51-5P |
| | | | 203929-61-7P |
| | | | 203929-70-8P |
| | | | 228869-44-1P |

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of phthalazines)

| | | | |
|----|---------------|--|--------------|
| IT | 86-54-4P | 269-50-1P, 1,3-Dioxolo[4,5-g]phthalazine | 1133-73-9P |
| | 2258-88-0P | 3306-76-1P | 3682-15-3P |
| | 5439-98-5P | 5441-28-1P | 6091-81-2P |
| | 7188-22-9P | 10089-99-3P | 10132-02-2P |
| | 13580-86-4P | 13580-88-6P | 13705-95-8P |
| | 16676-79-2P | 17045-94-2P | 17045-95-3P |
| | 18584-50-4P | 18584-52-6P | 18584-53-7P |
| | 18640-46-5P | 18697-31-9P | 21948-84-5P |
| | 24129-10-0P | 24953-61-5P | 24953-63-7P |
| | 25131-53-7P | 25732-39-2P | 25732-41-6P |
| | 26641-43-0P | 28081-56-3P | 29415-71-2P |
| | 38933-79-8P | 39794-28-0P | 39794-29-1P |
| | 49572-99-8P | 51334-85-1P | 51935-42-3P |
| | 57835-94-6P | 59283-65-7P | 59908-32-6P |
| | 62645-07-2P | 63536-23-2P | 63536-29-8P |
| | 63536-36-7P | 66859-14-1P | 68775-90-6P |
| | 73662-08-5P | 73662-09-6P | 73662-10-9P |
| | 76240-47-6P | 76462-35-6P | 76462-36-7P |
| | 76972-84-4P | 76972-85-5P | 81214-62-2P |
| | 82908-80-3P | 84257-71-6P | 86355-25-1P |
| | 87166-61-8P | 87255-77-4P | 89898-93-1P |
| | 89939-65-1P | 90876-71-4P | 93517-74-9P |
| | 93517-77-2P | 94106-83-9P | 95647-35-1P |
| | 98329-37-4P | 98670-35-0P | 98670-36-1P |
| | 99161-51-0P | 99185-48-5P | 100139-18-2P |
| | 100448-26-8P | 100448-27-9P | 100448-47-3P |
| | 100541-08-0P | 100962-00-3P | 101494-94-4P |
| | 102072-84-4P, | 5-Phthalazinamine | 103038-14-8P |
| | 103286-06-2P | 103286-07-3P | 103286-08-4P |
| | 103286-26-6P | 103286-28-8P | 103286-29-9P |
| | 105702-06-5P | 108618-32-2P | 110175-26-3P |
| | 112633-91-7P | 113222-30-3P | 121258-89-7P |
| | 122665-88-7P | 124397-50-8P | 124433-94-9P |
| | | | 100448-48-4P |
| | | | 101495-53-8P |
| | | | 101721-36-2P |
| | | | 103286-05-1P |
| | | | 103286-11-9P |
| | | | 103286-30-2P |
| | | | 110704-04-6P |
| | | | 122665-86-5P |
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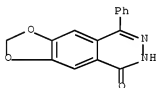
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|--------------|--|-------------------------|--------------|--------------|
| 126081-03-6P | 126278-18-0P | 126650-65-5P | 129221-92-7P | 132960-22-6P |
| 132960-23-7P | 134926-55-9P | 134926-67-3P | 134926-68-4P | 135033-30-6P |
| 135033-31-7P | 135033-32-8P | 135033-33-9P | 135033-34-0P | 135033-35-1P |
| 136610-31-6P | 136610-32-7P | 136610-33-8P | 137207-76-2P | 137381-09-0P |
| 137381-69-2P | 137382-01-5P | 137382-07-1P | 137382-08-2P | 137382-09-3P |
| 137382-45-7P | 137382-60-6P | 137387-90-7P | 155936-76-8P | 155936-78-0P |
| 155937-28-3P | 156020-35-8P | 159211-19-5P | 163120-65-8P | 163120-66-9P |
| 170373-52-1P | 170940-78-0P, 1-Phthalazinecarboxamide | | | 171084-38-1P |
| 171084-39-2P | 173463-56-4P | 173463-57-5P | 173463-58-6P | |
| 173463-60-0P | 173463-61-1P | 173463-62-2P | 173463-63-3P | 173605-15-7P |
| 178309-35-8P | 178309-36-9P | 180293-88-3P | 182683-72-3P | 184474-93-9P |
| 189213-64-7P | 201531-14-8P | 203929-72-0P | 203929-74-2P | 203929-76-4P |
| 203929-77-5P | 203929-78-6P | 203929-79-7P | 203929-80-0P | 203929-81-1P |
| 203929-82-2P | 203929-83-3P | 203929-84-4P | 203929-85-5P | 203929-86-6P |
| 203929-87-7P | 203929-88-8P | 203929-89-9P | 203929-90-2P | 203929-91-3P |
| 204520-35-4P | 210166-64-6P | 210166-74-8P | 212141-54-3P | 212141-72-5P |

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of phthalazines)

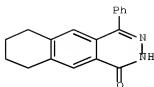
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| IT | 212142-91-1P | 212142-96-6P | 213765-59-4P | 219966-13-9P | 220411-63-2P |
| | 220411-64-3P | 220411-65-4P | 220411-66-5P | 220411-67-6P | 220411-68-7P |
| | 221632-80-0P | 221632-81-1P | 221632-83-3P | 221632-85-5P | 221632-86-6P |
| | 226385-56-8P | 226385-61-1P | 226385-64-4P | 226385-65-5P | 226995-82-0P |
| | 226995-84-2P | 226995-85-3P | 226995-86-4P | 226995-87-5P | 239077-04-4P |
| | 247256-15-1P | 247256-16-2P | 284031-00-1P | 284031-06-7P | 295780-86-8P |
| | 295793-48-5P | 297132-09-3P | 297132-10-6P | 297132-11-7P | |
| | 311339-03-4P | 313505-06-5P | 315678-22-9P | 343600-10-2P | 343945-05-1P |
| | 343965-02-6P | 350690-08-3P | 350690-10-7P | 350690-11-8P | 350690-12-9P |
| | 350690-14-1P | 350690-15-2P | 361364-46-7P | 412339-45-8P | 412340-49-9P |

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of phthalazines)

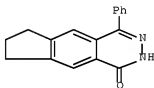
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|-----|---|-----------------|
| IT | 295793-36-1 | |
| RL: | RCT (Reactant); RACT (Reactant or reagent) | |
| | (preparation of phthalazines) | |
| RN | 295793-36-1 | HCAPLUS |
| CN | 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-phenyl- | (CA INDEX NAME) |



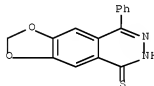
| | | |
|-----|---|-----------------|
| IT | 173463-59-7P | |
| RL: | RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) | |
| | (preparation of phthalazines) | |
| RN | 173463-59-7 | HCAPLUS |
| CN | Benzo[g]phthalazin-1(2H)-one, 6,7,8,9-tetrahydro-4-phenyl- | (CA INDEX NAME) |



IT 173463-57-5P 295793-48-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of phthalazines)
 RN 173463-57-5 HCAPLUS
 CN 1H-Cyclopenta[g]phthalazin-1-one, 2,6,7,8-tetrahydro-4-phenyl- (CA INDEX NAME)



RN 295793-48-5 HCAPLUS
 CN 1,3-Dioxolo[4,5-g]phthalazine-5(6H)-thione, 8-phenyl- (CA INDEX NAME)



REFERENCE COUNT: 384 THERE ARE 384 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L55 ANSWER 11 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2003:928884 HCAPLUS [Full-text](#)
 DOCUMENT NUMBER: 140:156731
 TITLE: 1-Aryl-6,7-methylenedioxy-3H-quinazolin-4-ones as anticonvulsant agents
 AUTHOR(S): Zappala, Maria; Grasso, Silvana; Micale, Nicola; Zuccala, Giuseppe; Menniti, Frank S.; Ferreri, Guido; De Sarro, Giovambattista; De Micheli, Carlo
 CORPORATE SOURCE: Dipartimento Farmaco-Chimico, Universita di Messina, Messina, 98168, Italy
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2003), 13(24), 4427-4430
 CODEN: BMCLEB; ISSN: 0960-894X

PUBLISHER: Elsevier Science B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 140:156731
 ED Entered STN: 28 Nov 2003

AB A set of novel 1-aryl-6,7-methylenedioxy-3H-quinazolin-4-(thi)ones has been designed and screened as anticonvulsant agents in DBA/2 mice. The new compds. are provided with anticonvulsant properties comparable to those of GYKI 52466. To clarify the mode of action, their affinity for the quinazolinone/2,3-benzodiazepine site of the AMPA receptor complex has been assayed.

CC 1-3 (Pharmacology)

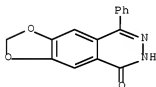
IT Section cross-reference(s): 27, 28
 253-52-1D, Phthalazine, derivs. 102771-26-6, GYKI 52466 197368-44-8
 197368-47-1 197368-49-3 250699-43-5 295793-36-1
295793-40-7 295793-49-6 656833-90-8D, derivs.
 656833-91-9D, derivs. 656834-00-3 656834-01-4 656824-02-5
656834-03-6 656834-04-7
 RL: PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study)

(arylmethylenedioxyquinazolinones as anticonvulsant agents)
 IT 295793-36-1 295793-40-7 295793-49-6
656834-02-5 656834-03-6 656834-04-7
 RL: PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study)

(arylmethylenedioxyquinazolinones as anticonvulsant agents)

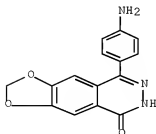
RN 295793-36-1 HCAPLUS

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-phenyl- (CA INDEX NAME)



RN 295793-40-7 HCAPLUS

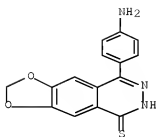
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(4-aminophenyl)- (CA INDEX NAME)



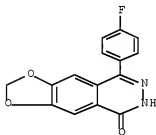
RN 295793-49-6 HCAPLUS

CN 1,3-Dioxolo[4,5-g]phthalazine-5(6H)-thione, 8-(4-aminophenyl)- (CA INDEX NAME)

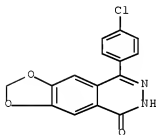
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RN 656834-02-5 HCAPLUS

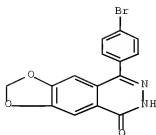
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(4-fluorophenyl)- (CA INDEX
NAME)

RN 656834-03-6 HCAPLUS

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(4-chlorophenyl)- (CA INDEX
NAME)

RN 656834-04-7 HCAPLUS

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(4-bromophenyl)- (CA INDEX
NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L55 ANSWER 12 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:91244 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 139:62588

TITLE: Characterization of the mechanism of anticonvulsant activity for a selected set of putative AMPA receptor antagonists

AUTHOR(S): Grasso, Silvana; Micale, Nicola; Zappala, Maria; Galli, Alessandro; Costagli, Chiara; Menniti, Frank S.; De Micheli, Carlo

CORPORATE SOURCE: Dipartimento Farmaco-Chimico, Universita di Messina, Messina, 98168, Italy

SOURCE: Bioorganic & Medicinal Chemistry Letters (2003), 13(3), 443-446

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 06 Feb 2003

AB A selected set of 1-aryl-7,8-methylenedioxy-2,3-benzodiazepin-4-ones and their analogs were evaluated for their ability to bind the competitive and noncompetitive sites of the AMPA receptors complex as well as to the glycine site of the NMDA receptors. The results put in evidence that most of the test compds., despite a close structural similarity with GYKI 52466, possess a significantly different pharmacol. profile.

CC 1-3 (Pharmacology)

IT 197368-49-3 197368-92-6 250699-34-4 [295793-40-7](#)

[295793-45-2](#) 343870-22-4 473451-53-5 473451-54-6

552290-38-7 552290-39-8 552290-40-1

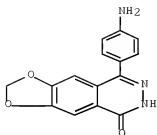
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(mechanism of anticonvulsant activity for putative AMPA receptor antagonists)

IT [295793-40-7](#) [295793-45-2](#)

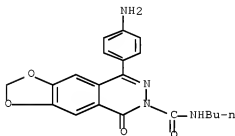
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(mechanism of anticonvulsant activity for putative AMPA receptor antagonists)

RN 295793-40-7 HCAPLUS

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(4-aminophenyl)- (CA INDEX NAME)



RN 295793-45-2 HCAPLUS
 CN 1,3-Dioxolo[4,5-g]phthalazine-6(5H)-carboxamide,
 8-(4-aminophenyl)-N-butyl-5-oxo- (CA INDEX NAME)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L55 ANSWER 13 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:747676 HCAPLUS Full-text

DOCUMENT NUMBER: 132:30247

TITLE: Synthesis of 2-[2-(1-imidazolyl)ethyl]-4-phenylcycloalka[g]phthalazin-1(2H)-ones as thromboxane A2 synthase inhibitors

AUTHOR(S): Haider, Norbert; Hartmann, Rolf W.; Steinwender, Andreas

CORPORATE SOURCE: Institute Pharmaceutical Chemistry, Univ. Vienna, Vienna, A-1090, Austria

SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1999), 332(11), 408-409

CODEN: ARPMAS; ISSN: 0365-6233

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 24 Nov 1999

AB A series of 2-[2-(1-imidazolyl)ethyl]-4-phenylcycloalka[g]phthalazin-1(2H)-ones with variable cycloalkene ring size was prepared and tested in vitro for thromboxane A2 synthase inhibitory activity.

CC 1-1 (Pharmacology)

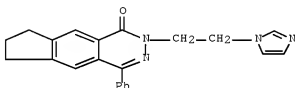
IT 119-39-1P, Phthalazinone 137381-09-0P 252662-91-2P

252662-92-3P 252662-93-4P 252662-94-5P

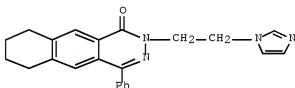
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

BIOL (Biological study); PREP (Preparation); USES (Uses)
 (synthesis of 2-[2-(1-imidazolyl)ethyl]-4-phenylcycloalka[g]phthalazin-
 1(2H)-ones as thromboxane A2 synthase inhibitors)

IT 252662-91-2P 252662-92-3P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological
 study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
 BIOL (Biological study); PREP (Preparation); USES (Uses)
 (synthesis of 2-[2-(1-imidazolyl)ethyl]-4-phenylcycloalka[g]phthalazin-
 1(2H)-ones as thromboxane A2 synthase inhibitors)
 RN 252662-91-2 HCAPLUS
 CN 1H-Cyclopenta[g]phthalazin-1-one, 2,6,7,8-tetrahydro-2-[2-(1H-imidazol-1-
 yl)ethyl]-4-phenyl- (CA INDEX NAME)

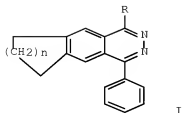


RN 252662-92-3 HCAPLUS
 CN Benzo[g]phthalazin-1(2H)-one, 6,7,8,9-tetrahydro-2-[2-(1H-imidazol-1-
 yl)ethyl]-4-phenyl- (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L55 ANSWER 14 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1996:577161 HCAPLUS Full-text
 DOCUMENT NUMBER: 125:300931
 ORIGINAL REFERENCE NO.: 125:56327a,56330a
 TITLE: Synthesis of g-annelated phthalazines as potential
 blood platelet aggregation inhibitors
 AUTHOR(S): Haider, Norbert; Steinwender, Andreas
 CORPORATE SOURCE: Institute Pharmaceutical Chemistry, University Vienna,
 Vienna, A-1090, Austria
 SOURCE: Scientia Pharmaceutica (1996), 64(3/4), 399-405
 CODEN: SCPHA4; ISSN: 0036-8709
 PUBLISHER: Oesterreichische Apotheker-Verlagsgesellschaft
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 ED Entered STN: 27 Sep 1996
 GI



AB The phthalazines I (n = 1-4; R = NHR₁; R₁ = 3-ClC₆H₄, CH₂CMe₃) were prepared from the corresponding phthalazinones via the chloro compds. I (n = 1-4; R = Cl).

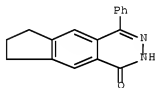
CC 28-15 (Heterocyclic Compounds (More Than One Hetero Atom))

IT 108-42-9, 3-Chloroaniline 5813-64-9 [173463-57-5](#)
[173463-59-7](#) 173463-61-1 173463-63-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of phthalazines)

IT [173463-57-5](#) [173463-59-7](#)
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of phthalazines)

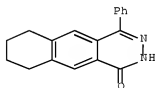
RN 173463-57-5 HCAPLUS

CN 1H-Cyclopenta[g]phthalazin-1-one, 2,6,7,8-tetrahydro-4-phenyl- (CA INDEX NAME)



RN 173463-59-7 HCAPLUS

CN Benzo[g]phthalazin-1(2H)-one, 6,7,8,9-tetrahydro-4-phenyl- (CA INDEX NAME)



ORIGINAL REFERENCE NO.: 52:15487a-f

TITLE: Polycyclic compounds. IV.
2,9-Dimethyl-7,14-dioxo-5,12-dihydropentacene-6,13-quinone and 5,12-dihydrotetracene

AUTHOR(S): Buchta, Emil; Egger, Hermann

CORPORATE SOURCE: Univ. Erlangen, Germany

SOURCE: Chemische Berichte (1957), 90, 2760-3

CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

ED Entered STN: 22 Apr 2001

AB cf. C.A. 51, 10466g. 2,5-Bis(2,5-dimethylbenzoyl)hydroquinone (I) (5 g.) heated to 340° and the sublimate recrystd. from 70% EtOH gave 900 mg. 2,5-Me2C6H3CO2H, needles, m. 132°. 2,5-Bis(2,5-dimethylbenzoyl)-p-quinone (6 g.) and 3 g. glass powder heated to 380°, kept 30-40 min. at this temperature, cooled, powdered, and sublimed at 0.4 mm. gave to 250° I and from 350-60° a glassy red product which extracted twice with Et2O and recrystd. from xylene gave 2,9-dimethyl-7,14-dioxo-5,12-dihydropentacene-6,13-quinone, light brown needles, m. 384-6°; it gave a blue solution with intense red fluorescence in concentrated H2O4. o-C6H4(CH2Br)2 (52 g.) in 250 cc. absolute EtOH, 63 g. [CH(CO2Et)2]2 in 300 cc. absolute EtOH, and 9.5 g. Na in 140 cc. EtOH heated 6 hrs. in an autoclave to 130° and concentrated, the residue dissolved in a little H2O, acidified with dilute H2SO4, and extracted with Et2O, and the extract worked up gave 70 g. tetra-Et 1,2,3,4-tetrahydronaphthalene-2,2,3,3-tetracarboxylate (II), viscous oil, b0.01 170°. II (42 g.) in 60 cc. MeOH refluxed with 100 cc. 40% KOH in MeOH, the MeOH distilled, the residue dissolved in 150 cc. H2O, the solution filtered, acidified with 2N H2SO4, and extracted with Et2O, the extract dried and evaporated, and the oily residue heated to 180-90° until the CO2 and H2O elimination ceased, cooled, and triturated with Et2O gave 14g. 1,2,3,4-tetrahydronaphthalene-2,3-dicarboxylic acid anhydride (III), m. 184°. III (5 g.) in 150 cc. dry C6H6 treated with 6.7 g. powdered AlCl3, refluxed 2 hrs., poured into ice and concentrated HCl, and filtered yielded 6.5 g. 2-benzoyl-1,2,3,4-tetrahydronaphthalene-3-carboxylic acid (IV), m. 182-4° (xylene). IV (2 g.) in 20 cc. 92% N2H4.H2O refluxed 1 hr. and cooled gave 1.5 g. 1-phenyl-4-hydroxy-4a,9,9a,10-tetrahydro-2,3-diazaanthracene, m. 198° (98% EtOH). Zn dust (30 g.), 3 g. HgCl2 in 150 cc. H2O, and 5 cc. concentrated HCl shaken 5 min., the solution decanted, the residue refluxed 24 hrs. with 20 cc. H2O and 45 cc. concentrated HCl, 10 g. IV, 150 cc. PhMe, and 3 cc. glacial AcOH while adding at 6 hr.-intervals 20-cc. portions of concentrated HCl and cooled, and the PhMe layer evaporated yielded 8.6 g. 2-PhCH2 analog (V) of IV, m. 146-8° (50% AcOH). V (2 g.) and 3 g. NaCl heated under a stream of N at 310° until the elimination of H2O ceased, cooled, dissolved in dilute HCl, and filtered, and the residue triturated with Et2O gave 1 g. 5,12-dihydrotetracene, needles, m. 208-9° (xylene).

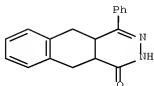
CC 10 (Organic Chemistry)

IT 610-72-0P, Benzoic acid, 2,5-dimethyl- 959-02-4P, Naphthacene,
5,12-dihydro- 29811-05-0P, 2,3-Naphthalenedicarboxylic anhydride,
1,2,3,4-tetrahydro- 76044-99-0P, 2,2,3,3-Naphthalenetetracarboxylic
acid, 1,4-dihydro-, tetraethyl ester 101723-54-0P, 2-Naphthoic acid,
3-benzoyl-1,2,3,4-tetrahydro- 101789-59-7P, 2-Naphthoic acid,
3-benzyl-1,2,3,4-tetrahydro- ~~109892-05-9P~~,
Benzo[g]phthalazin-1-ol, 4a,5,10,10a-tetrahydro-4-phenyl- 114722-26-8P,
5,6,12,13(7H,14H)-Pentacetetetrone, 3,10-dimethyl-
RL: PREP (Preparation)
(preparation of)

IT ~~109892-05-9P~~, Benzo[g]phthalazin-1-ol,
4a,5,10,10a-tetrahydro-4-phenyl-
RL: PREP (Preparation)
(preparation of)

RN 109892-05-9 HCAPLUS

CN Benzo[g]phthalazin-1(2H)-one, 4a,5,10,10a-tetrahydro-4-phenyl- (CA INDEX NAME)



L55 ANSWER 16 OF 24 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1931:16478 HCAPLUS Full-text

DOCUMENT NUMBER: 25:16478

ORIGINAL REFERENCE NO.: 25:1821h-i,1822a

TITLE: Pyromellitic acid. Benzodiketohydrindene and benzodipyridazine derivatives

AUTHOR(S): Seka, Reinhard; Sedlatschek, Hans; Preissecker, Heinrich

SOURCE: Monatshefte fuer Chemie (1931), 57, 86-96

CODEN: MOCMB7; ISSN: 0026-9247

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

ED Entered STN: 16 Dec 2001

AB O(CO)2C6H2(CO)2O (I) and quinaldine, heated at 250° until the mass is solid, give the condensation product (II), C30H16O4N2, dark reddish brown, decomps. 265°, insol. in EtOH, and the yellow-brown, EtOH-soluble compound, C20H11O6N, decomps. about 125°. Sulfonation of II with 50% oleum at 170° gives a product similar to quinoline yellow, which dyes wool and silk a pure yellow. I and α -C10H7NH2 give pyromellitic dinaphthylimide, m. 431°. N2H4.H2O (4 mols.) gives the dihydrazide, light yellow, decomps. about 450°; its tetra-Ac derivative m. 235-8°. 1,4,2,5-Bz2C6H2(CO2H)2 and 10 mols. N2H4.H2O in absolute EtOH, heated 24 hrs. at 120°, give 90% of 1,6-diphenyl-4,9-dihydroxybenzodipyridazine, carbonizes at 445°; 1,5,2,4-Bz2C6H2(CO2H)2 and 6 mols. N2H4.H2O give the 1,9-diphenyl-4,6-dihydroxy derivative, decomps. 430°. (MeC5H4CO)2C6H2(CO2H)2 and N2H4.H2O give the 1,9-dixylyl-4,6-dihydroxy derivative, carbonizes at a high temperature 2-Benzoylanthraquinone-3-carboxylic acid and 3.8 mols. N2H4.H2O in absolute EtOH, heated 9 hrs. at 120°, give the hydrazide, light yellow, decomps. 374°. 1,2,4,5-C6H2(COCl)4 and MeONa in C6H6 give 88% of tetra-Me pyromellitate, m. 138°; the tetra-Ph ester, m. 179.5°, results in 24% yields.

CC 10 (Organic Chemistry)

IT 4760-87-6P, Pyridazo[4,5-g]phthalazine-1,4,6,9(2,3,7,8)-tetrone
 31663-83-9P, Pyromellitide, N,N'-di-1-naphthyl- 161535-66-6P,
 Pyridazo[4,5-g]phthalazine-1,6-diol, 4,9-diphenyl- 161535-67-7P,
 Pyridazo[4,5-g]phthalazine-1,9-diol, 4,6-diphenyl- 853118-02-2P,
 Pyridazo[4,5-g]phthalazine-1,4,6,9(2,3,7,8)-tetrone, 2,3,7,8-tetraacetyl-
~~858920-38-2P~~, Naphtho[2,3-g]phthalazine-6,11-dione,
 1-hydroxy-4-phenyl-

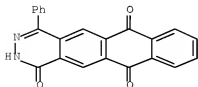
RL: PREP (Preparation)
(preparation of)

IT ~~858920-38-2P~~, Naphtho[2,3-g]phthalazine-6,11-dione,
 1-hydroxy-4-phenyl-

RL: PREP (Preparation)
(preparation of)

10/772,445

RN 858020-38-9 HCAPLUS
CN Naphtho[2,3-g]phthalazine-1,6,11(2H)-trione, 4-phenyl- (CA INDEX NAME)



=> d 17

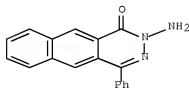
YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS, CAOLD, CHEMCATS, CHEMINFORMRX' -
CONTINUE? (Y)/N:y

L55 ANSWER 17 OF 24 CAOLD COPYRIGHT 2008 ACS on STN
AN CA52:15486i CAOLD
TI unsatd. hydrocarbons
AU Kotlyarevskii, I. L.; Zanina, A. S.; Lipovich, V. G.
IT 959-02-4 1076-61-5 1559-81-5 1680-51-9 2809-64-5
3877-19-8 21564-92-1 29811-05-0 76044-99-0 101723-54-0 101789-59-7
109857-05-9 114722-26-8

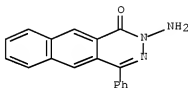
=> d ide 18-20

YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS, CAOLD, CHEMCATS, CHEMINFORMRX' -
CONTINUE? (Y)/N:y

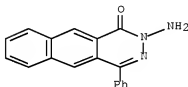
L55 ANSWER 18 OF 24 CHEMCATS COPYRIGHT 2008 ACS on STN
Accession No. (AN): 2043513538 CHEMCATS
Catalog Name (CO): Ryan Scientific Screening Library
Publication Date (PD): 25 Jan 2008
Order Number (ON): AK-830/13217101
Chemical Name (CN): Benzo[g]phthalazin-1(2H)-one, 2-amino-4-phenyl-
CAS Registry No. (RN): 445224-50-0
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :



L55 ANSWER 19 OF 24 CHEMCATS COPYRIGHT 2008 ACS on STN
 Accession No. (AN): 2020466079 CHEMCATS
 Catalog Name (CO): Interchim Intermediates
 Publication Date (PD): 18 Feb 2008
 Order Number (ON): AK-830/13217101
 Chemical Name (CN): Benzo[g]phthalazin-1(2H)-one, 2-amino-4-phenyl-
 CAS Registry No. (RN): 445224-50-0
 Supplementary Term (ST): CHEMICAL LIBRARY
 Structure :



L55 ANSWER 20 OF 24 CHEMCATS COPYRIGHT 2008 ACS on STN
 Accession No. (AN): 2017061712 CHEMCATS
 Catalog Name (CO): Compounds For Screening
 Publication Date (PD): 2 Oct 2008
 Order Number (ON): AK-830/13217101
 Chemical Name (CN): 2-amino-4-phenylbenzo[g]phthalazin-1(2H)-one
 CAS Registry No. (RN): 445224-50-0
 Supplementary Term (ST): CHEMICAL LIBRARY
 Structure :



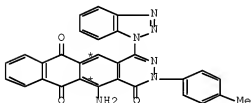
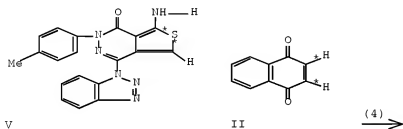
=> d bib ab hit 21-24

YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS, CAOLD, CHEMCATS, CHEMINFORMRX' -
 CONTINUE? (Y)/N:y

L55 ANSWER 21 OF 24 CHEMINFORMRX COPYRIGHT 2008 FIZ CHEMIE on STN

AN 200534151 CHEMINFORMRX [Full-text](#)
 TI Studies with Condensed Thiophenes: Reactivity of Condensed Aminothiophenes
 Toward Carbon and Nitrogen Electrophiles.
 AU AL-SALEH, B.; ABDELKHALIK, M. M.; EL-APASERY, M. A.; ELNAGDI, M. H.
 CS Dep. Chem., Fac. Sci., Univ. Kuwait, Safat 13060, Kuwait
 SO J. Chem. Res.(1), 23-26 (2005)
 CODEN: JCROA4 ISSN: 0308-2342
 LA English

RX(4) OF 17 I + B ==> J

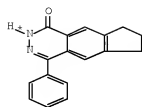


YIELD 56.0%

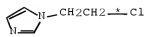
RX(4) RCT V, 727009
 II, 1180 (130-15-4)
 SOL 81 (64-17-5), EtOH
 PRO VI, [1097121](#)
 YDS 56.0 %
 T.KW REFLUX
 KW aromatisation; alkylation; C-alkylation
 NTE reaction:V (II) -> VI, example: 2

L55 ANSWER 22 OF 24 CHEMINFORMRX COPYRIGHT 2008 FIZ CHEMIE on STN
 AN 200007133 CHEMINFORMRX [Full-text](#)
 TI Synthesis of 2-[2-(1-Imidazolyl)ethyl]-4-phenylcycloalka[g]phthalazin-
 1(2H)-ones as Thromboxane A2 Synthase Inhibitors.
 AU HAIDER, N.; HARTMANN, R. W.; STEINWENDER, A.
 CS Inst. Pharm. Chem., Univ. Wien, A-1090 Wien, Austria
 SO Arch. Pharm. (Weinheim, Ger.), 332(11), 408-409 (1999)
 CODEN: ARPMAS ISSN: 0365-6233
 LA English
 AB The title compounds (III) show thromboxane A2 synthase inhibitory activity
 which decreases with increasing ring size.

RX(1) OF 3 A + B ==> C

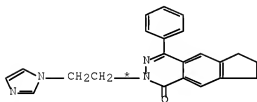


I



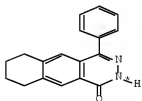
II

(1) →

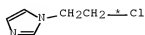
III
YIELD 68.0%

RX(1) RCT I, 447980
 II, 720168
 RGT 1163 (7646-69-7), NaH
 SOL 76 (68-12-2), DMF
 PRO III, 720169
 YDS 68.0 %
 T 25.0 - 70.0 Cel
 KW alkylation; N-alkylation
 NTE reaction:I (II) -> III, example: 1

RX(2) OF 3 F + B ==> G

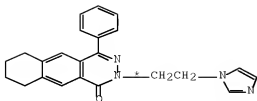


I



II

(2) →

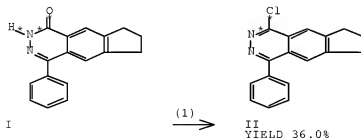


III
YIELD 70.0%

RX(2) RCT I, 527603
II, 720168
RGT 1163 (7646-69-7), NaH
SOL 76 (68-12-2), DMF
PRO III, 720170
YDS 70.0 %
T 25.0 - 70.0 Cel
KW alkylation; N-alkylation
NTE reaction: I (II) -> III, example: 2

L55 ANSWER 23 OF 24 CHEMINFORMRX COPYRIGHT 2008 FIZ CHEMIE on STN
AN 199718188 CHEMINFORMRX Full-text
TI Synthesis of g-Annelated Phthalazines as Potential Blood Platelet
Aggregation Inhibitors.
AU HAIDER, N.; STEINWENDER, A.
CS Inst. Pharm. Chem., Univ. Wien, A-1090 Wien, Austria
SO Sci. Pharm., 64(3), 399-405 (1996)
CODEN: SCPHA4 ISSN: 0036-8709
LA English
AB A series of cycloalkene-fused 1-arylamino- and 1-alkylamino-4-
phenylphthalazines (IV) (8 examples) is prepared by amination of readily
achieved chloro compounds (II). Compounds (IV) represent a novel type of
analogues of known antiaggregatory agents, however, only compound (IIIa)
exhibits some platelet antiaggregatory potency.

RX(1) OF 11 A ==> B...



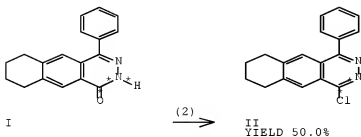
RX(1) RCT I, 447880
RGT 181 (10025-87-3), POC13
63 (91-66-7), Ph-Net2
PRO II, 527602
YDS 36.0 %
T 90.0 Cel

10/772,445

KW aromatisation; halogenation; C-halogenation; chlorination;
alkylation

NTE reaction:I -> II, example: 1

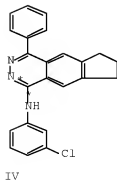
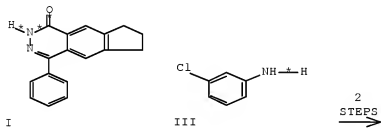
RX(2) OF 11 E ==> F...



RX(2) RCT I, 527603
RGT 181 (10025-87-3), POCl3
63 (91-66-7), Ph-Net2
PRO II, 527604
YDS 50.0 %
T 90.0 Cel
KW aromatisation; halogenation; C-halogenation; chlorination;
alkylation
NTE reaction:I -> II, example: 2

RX(8) OF 11 COMPOSED OF RX(1), RX(4)

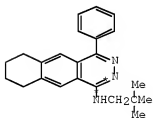
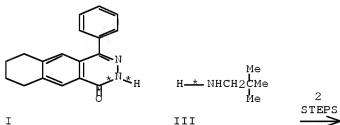
RX(8) A + I ==> J



RX(1) RCT I, 447880
 RGT 181 (10025-87-3), POC13
 63 (91-66-7), Ph-NEt2
 PRO II, 527602
 YDS 36.0 %
 T 90.0 Cel
 KW aromatisation; halogenation; C-halogenation; chlorination;
 alkylation
 NTE reaction:I -> II, example: 1
 RX(4) RCT II, 527602
 III, 14699 (108-42-9)
 SOL 80 (123-91-1), dioxane
 PRO IV, 527606
 T 130.0 Cel
 KW arylation
 NTE [sealed tube]; reaction:II (III) -> IV, example: 1

RX(9) OF 11 COMPOSED OF RX(2), RX(5)

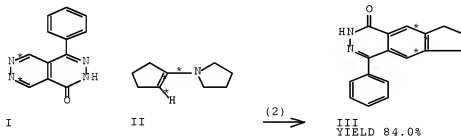
RX(9) E + L ==> M



RX(2) RCT I, 527603
 RGT 181 (10025-87-3), POC13
 63 (91-66-7), Ph-NEt2
 PRO II, 527604
 YDS 50.0 %
 T 90.0 Cel
 KW aromatisation; halogenation; C-halogenation; chlorination;
 alkylation
 NTE reaction:I -> II, example: 2
 RX(5) RCT II, 527604
 III, 370369

```
SOL 80 (123-91-1), dioxane
PRO IV, 527607
T 100.0 Cel
KW arylation
NTE [sealed tube]; reaction:II (III) -> IV, example: 2
```

ANSWER 24 OF 24 CHEMINFORMRX COPYRIGHT 2008 FIZ CHEMIE on STN
AN 199612174 CHEMINFORMRX Full-Text
TI Inverse-Electron-Demand Diels-Alder Reactions of Condensed Pyridazines.
Part 8. Convenient Synthesis of Cycloalkene-Fused Phthalazinones.
AU HAIDER, N.
CS Inst. Pharm. Chem., Univ. Wien, A-1090 Wien, Austria
SO Heterocycles, 41(11), 2519-2525 (1995)
CODEN: HTCYAM ISSN: 0385-5414
LA English
AB Cycloalkene-anellated phthalazin-1(2H)-ones (III) are easily prepared by an
inverse-electron-demand Diels-Alder reaction of the pyridazino[4,3-b]pyridazine (I)
with the enamines (II) followed by acid-catalyzed aromatization of
intermediates (IV). C4-Substituted phthalazinones are key compounds in the
synthesis of platelet aggregation or thromboxane A2 synthetase inhibitors.

$$RX(2) \quad OF \quad 4 \quad G \quad + \quad B \quad ==> \quad H$$


```

RX(2)      RCT      I, 447879
              II, 17585 (7148-07-4)
              STAGE(1)
                SOL    80 (123-91-1), dioxane
                T.KW    REFLUX
                TIM      1.0 hr
              STAGE(2)
                RGT      3 (64-19-7), AcOH
                SOL    182 (71-23-8), ProH
                T.KW    REFLUX
                TIM      24 hr
              PRO      III, 447880
              YDS      84.0 %
              KW        aromatisation; addition; olefination
              NTE       reaction: I + II -> III, example: 2
              CMT       #E0100:(100% e.e.[92% d.e.])

```

=> fil beilst
 FILE 'BEILSTEIN' ENTERED AT 15:50:54 ON 04 DEC 2008
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FILE LAST UPDATED ON April 1, 2008

FILE COVERS 1771 TO 2008.

*** FILE CONTAINS 10.322,808 SUBSTANCES ***

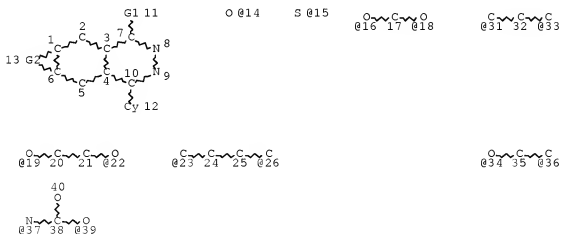
>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For more detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

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 * ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. *
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>>> Price change as of January 1st, 2008: Connect Time and Structure Search fees re-introduced. See NEWS and HELP COST <<<

=> d que stat 139
 L13 STR



VAR G1=14/15

VAR G2=16-6 18-1/19-6 22-1/31-6 33-1/23-6 26-1/34-6 36-1/36-6 34-1/37-6 3

9-1/39-6 37-1

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 14
CONNECT IS E1 RC AT 15
CONNECT IS E1 RC AT 40
DEFAULT MLEVEL IS ATOM
GGCAT IS UNS AT 12
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 36

STEREO ATTRIBUTES: NONE

L39 33 SEA FILE=BEILSTEIN SSS FUL L13

100.0% PROCESSED 3620 ITERATIONS

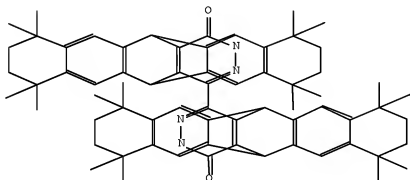
33 ANSWERS

SEARCH TIME: 00.00.05

=> d ide l39 1

L39 ANSWER 1 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN): 11079041
 Chemical Name (CN): 1,1'-bi(5'',6'',7,7'',8,8'',9,10-octahydro-5'',5'',7,7,8'',8''10,10-octamethyl-5,12-<2'',3''>naphthaleno-2,3-diazatetracenyl)-4,4' (3H,3'H)-dione
 Molec. Formula (MF): C68 H78 N4 O2
 Molecular Weight (MW): 983.39
 Lawson Number (LN): 30560
 Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 9259960
 Tautomer ID (TAUTID): 10315765
 Entry Date (DED): 2008/04/19
 Update Date (DUPD): 2008/04/19



Field Availability:

| Code | Name | Occurrence |
|--------|----------------------------|------------|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 1 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |
| NMR | Nuclear Magnetic Resonance | 4 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|------|------|------------|
|------|------|------------|

```
=====
RX           Reaction Documents                2
RXREA        Substance is Reaction Reactant    1
RXPRO        Substance is Reaction Product     1
```

=> d rx l39 1

L39 ANSWER 1 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:

```
RX
  Reaction ID (.ID):          10780544
  Reactant BRN (.RBRN):      11078905
  Reactant (.RCT):           1,1'-bi(5'',6'',7,7'',8,8'',9,10-octahydro
                              -5'',5'',7,7,8'',8'',10,10-octamethyl-4-me
                              thoxy-5,12-<2'',3''>naphthaleno-2,3-diazat
                              etracenyl)
  Product BRN (.PBRN):       11079041
  Product (.PRO):            1,1'-bi(5'',6'',7,7'',8,8'',9,10-octahydro
                              -5'',5'',7,7,8'',8''10,10-octamethyl-5,12-
                              <2'',3''>naphthaleno-2,3-diazatetracenyl)-
                              4,4' (3H,3'H)-dione
  No. of React. Details (.NVAR): 1
```

Reaction Details:

```
RX
  Reaction RID (.RID):        10780544.1
  Reaction Classification (.CL): Preparation
  Yield (.YDT):               100 percent (BRN=11079041)
  Reagent (.RGT):             HBr, AcOH
  Temperature (.T):           95 Cel
  Reference(s):
  1. Bouffard, Jean; Eaton, Robert F.; Mueller, Peter; Swager, Timothy M.,
    J. Org. Chem., CODEN: JOCEAH, SIR72(26), <2007>, 10166 - 10180;
    BABS-6716975
```

Reaction:

```
RX
  Reaction ID (.ID):          10780576
  Reactant BRN (.RBRN):      11079041
  Reactant (.RCT):           1,1'-bi(5'',6'',7,7'',8,8'',9,10-octahydro
                              -5'',5'',7,7,8'',8''10,10-octamethyl-5,12-
                              <2'',3''>naphthaleno-2,3-diazatetracenyl)-
                              4,4' (3H,3'H)-dione
  Product BRN (.PBRN):       11078937
  Product (.PRO):            1,1'-bi(4-chloro-5'',6'',7,7'',8,8'',9,10-
                              octahydro-5'',5'',7,7,8'',8'',10,10-octame
                              thyl-5,12-<2'',3''>naphthaleno-2,3-diazate
                              tracenyl)
  No. of React. Details (.NVAR): 1
```

Reaction Details:

```
RX
  Reaction RID (.RID):        10780576.1
  Reaction Classification (.CL): Preparation
  Yield (.YDT):               79 percent (BRN=11078937)
  Reagent (.RGT):             POC13
  Temperature (.T):           80 Cel
```

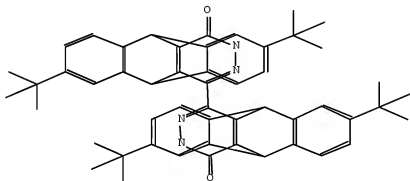
Reference(s):

1. Bouffard, Jean; Eaton, Robert F.; Mueller, Peter; Swager, Timothy M., J. Org. Chem., CODEN: JOCEAH, SIR72(26), <2007>, 10166 - 10180; BABS-6716975

=> d ide 139 2

L39 ANSWER 2 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN): 11074617
 Chemical Name (CN): 1,1'-bi(5'',6-di-tert-butyl-9,10-dihydro-9,10-<1'',2''>benzo-2,3-diazaanthracenyl)-4,4' (3H,3'H)-dione
 Molec. Formula (MF): C52 H54 N4 O2
 Molecular Weight (MW): 767.02
 Lawson Number (LN): 30564
 Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 9256297
 Tautomer ID (TAUTID): 10313539
 Entry Date (DED): 2008/04/19
 Update Date (DUPD): 2008/04/19



Field Availability:

| Code | Name | Occurrence |
|--------|-------------------|------------|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 1 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|-------|--------------------------------|------------|
| RX | Reaction Documents | 2 |
| RXREA | Substance is Reaction Reactant | 1 |
| RXPRO | Substance is Reaction Product | 1 |

=> d rx l39 2

L39 ANSWER 2 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:

RX

| | |
|--------------------------------|--|
| Reaction ID (.ID): | 10779415 |
| Reactant BRN (.RBRN): | 11074651 |
| Reactant (.RCT): | 1,1'-bi(5'',6-di-tert-butyl-9,10-dihydro-4-methoxy-9,10-<1'',2''>benzeno-2,3-diazaanthracenyl) |
| Product BRN (.PBRN): | 11074617 |
| Product (.PRO): | 1,1'-bi(5'',6-di-tert-butyl-9,10-dihydro-9,10-<1'',2''>benzeno-2,3-diazaanthracenyl)-4,4'-(3H,3'H)-dione |
| No. of React. Details (.NVAR): | 1 |

Reaction Details:

RX

| | |
|--------------------------------|---|
| Reaction RID (.RID): | 10779415.1 |
| Reaction Classification (.CL): | Preparation |
| Yield (.YDT): | 97 percent (BRN=11074617) |
| Reagent (.RGT): | HBr, AcOH |
| Temperature (.T): | 95 Cel |
| Reference(s): | 1. Bouffard, Jean; Eaton, Robert F.; Mueller, Peter; Swager, Timothy M., J. Org. Chem., CODEN: JOCEAH, SIR72(26), <2007>, 10166 - 10180; BABS-6716975 |

Reaction:

RX

| | |
|--------------------------------|--|
| Reaction ID (.ID): | 10779407 |
| Reactant BRN (.RBRN): | 11074617 |
| Reactant (.RCT): | 1,1'-bi(5'',6-di-tert-butyl-9,10-dihydro-9,10-<1'',2''>benzeno-2,3-diazaanthracenyl)-4,4'-(3H,3'H)-dione |
| Product BRN (.PBRN): | 11074271 |
| Product (.PRO): | 1,1'-bi(5'',6-di-tert-butyl-4-chloro-9,10-dihydro-9,10-<1'',2''>benzeno-2,3-diazaanthracenyl) |
| No. of React. Details (.NVAR): | 1 |

Reaction Details:

RX

| | |
|--------------------------------|---------------------------|
| Reaction RID (.RID): | 10779407.1 |
| Reaction Classification (.CL): | Preparation |
| Yield (.YDT): | 76 percent (BRN=11074271) |
| Reagent (.RGT): | POCl3 |

10/772,445

Temperature (.T):

60 Cel

Reference(s):

1. Bouffard, Jean; Eaton, Robert F.; Mueller, Peter; Swager, Timothy M.,
 J. Org. Chem., CODEN: JOCEAH, SIR72(26), <2007>, 10166 - 10180;
 BABS-6716975

=> d ide 139 3

L39 ANSWER 3 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN):

11065936

Chemical Name (CN):

1,1'-bi(9,10-dihydro-9,10-<1'',2''>benzo-
 -2,3-diazaanthracenyl)-4,4'(3H,3'H)-dione
 C36 H22 N4 O2

Molec. Formula (MF):

542.60

Molecular Weight (MW):

30560

Lawson Number (LN):

heterocyclic

Compound Type (CTYPE):

Constitution ID (CONSID):

9249543

Tautomer ID (TAUTID):

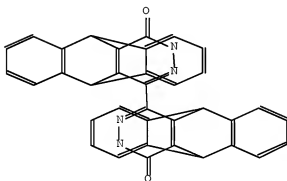
10311733

Entry Date (DED):

2008/04/19

Update Date (DUPD):

2008/04/19



Field Availability:

| Code | Name | Occurrence |
|--------|-------------------|------------|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 1 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|-------|--------------------------------|------------|
| RX | Reaction Documents | 3 |
| RXREA | Substance is Reaction Reactant | 2 |
| RXPRO | Substance is Reaction Product | 1 |

=> d rx l39 3

L39 ANSWER 3 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:

```

RX
  Reaction ID (.ID):          10776880
  Reactant BRN (.RBRN):      11065310
  Reactant (.RCT):           1,1'-bi(9,10-dihydro-4-methoxy-9,10-<1'',2
                              ''>benzeno-2,3-diazaanthracenyl)
  Product BRN (.PBRN):       11065936
  Product (.PRO):            1,1'-bi(9,10-dihydro-9,10-<1'',2''>benzeno
                              -2,3-diazaanthracenyl)-4,4'(3H,3'H)-dione
  No. of React. Details (.NVAR): 1

```

Reaction Details:

```

RX
  Reaction RID (.RID):        10776880.1
  Reaction Classification (.CL): Preparation
  Yield (.YDT):               91 percent (BRN=11065936)
  Reagent (.RGT):             HBr, AcOH
  Temperature (.T):           90 Cel
  Reference(s):
  1. Bouffard, Jean; Eaton, Robert F.; Mueller, Peter; Swager, Timothy M.,
    J. Org. Chem., CODEN: JOCEAH, SIR72(26), <2007>, 10166 - 10180;
    BABS-6716975

```

Reaction:

```

RX
  Reaction ID (.ID):          10777066
  Reactant BRN (.RBRN):      11065936
  Reactant (.RCT):           1,1'-bi(9,10-dihydro-9,10-<1'',2''>benzeno
                              -2,3-diazaanthracenyl)-4,4'(3H,3'H)-dione
  Product BRN (.PBRN):       11065026
  Product (.PRO):            1,1'-bi(4-bromo-9,10-dihydro-9,10-<1'',2''
                              >benzeno-2,3-diazaanthracenyl)
  No. of React. Details (.NVAR): 1

```

Reaction Details:

```

RX
  Reaction RID (.RID):        10777066.1
  Reaction Classification (.CL): Preparation
  Yield (.YDT):               39 percent (BRN=11065026)
  Reagent (.RGT):             POBr3
  Solvent (.SOL):             toluene
  Temperature (.T):           90 Cel
  Reference(s):
  1. Bouffard, Jean; Eaton, Robert F.; Mueller, Peter; Swager, Timothy M.,

```

J. Org. Chem., CODEN: JOCEAH, SIR72(26), <2007>, 10166 - 10180;
BABS-6716975

Reaction:

RX

Reaction ID (.ID): 10777065
 Reactant BRN (.RBRN): 11065936
 Reactant (.RCT): 1,1'-bi(9,10-dihydro-9,10-<1'',2''>benzeno-2,3-diazaanthracenyl)-4,4'-(3H,3'H)-dione
 Product BRN (.PBRN): 11064586
 Product (.PRO): 1,1'-bi(4-chloro-9,10-dihydro-9,10-<1'',2''>benzeno-2,3-diazaanthracenyl)
 No. of React. Details (.NVAR): 1

Reaction Details:

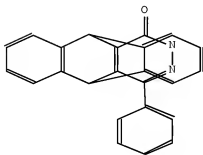
RX

Reaction RID (.RID): 10777065.1
 Reaction Classification (.CL): Preparation
 Yield (.YDT): 66 percent (BRN=11064586)
 Reagent (.RGT): POC13
 Temperature (.T): 90 Cel
 Reference(s):
 1. Bouffard, Jean; Eaton, Robert F.; Mueller, Peter; Swager, Timothy M.,
 J. Org. Chem., CODEN: JOCEAH, SIR72(26), <2007>, 10166 - 10180;
 BABS-6716975

=> d ide 139 4

L39 ANSWER 4 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN): 11028913
 Chemical Name (CN): 9,10-dihydro-4-phenyl-9,10-<1',2'>benzeno-2,3-diazaanthracen-1(2H)-one
 Molec. Formula (MF): C24 H16 N2 O
 Molecular Weight (MW): 348.40
 Lawson Number (LN): 28763
 Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 9218605
 Tautomer ID (TAUTID): 10299045
 Entry Date (DED): 2008/04/19
 Update Date (DUPD): 2008/04/19



Field Availability:

| Code | Name | Occurrence |
|--------|----------------------------|------------|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 1 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |
| NMR | Nuclear Magnetic Resonance | 4 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|-------|--------------------------------|------------|
| RX | Reaction Documents | 2 |
| RXREA | Substance is Reaction Reactant | 1 |
| RXPRO | Substance is Reaction Product | 1 |

=> d rx 139 4

L39 ANSWER 4 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:

RX
 Reaction ID (.ID): 10767049
 Reactant BRN (.RBRN): 11028325
 Reactant (.RCT): 9,10-dihydro-1-methoxy-4-phenyl-9,10-<1',2'
 '>benzeno-2,3-diazaanthracene
 Product BRN (.PBRN): 11028913
 Product (.PRO): 9,10-dihydro-4-phenyl-9,10-<1',2'>benzeno-
 2,3-diazaanthracen-1(2H)-one
 No. of React. Details (.NVAR): 1

Reaction Details:

RX
 Reaction RID (.RID): 10767049.1
 Reaction Classification (.CL): Preparation
 Yield (.YDT): 72 percent (BRN=11028913)
 Reagent (.RGT): HBr, AcOH
 Temperature (.T): 90 Cel
 Reference(s):
 1. Bouffard, Jean; Eaton, Robert F.; Mueller, Peter; Swager, Timothy M.,
 J. Org. Chem., CODEN: JOCEAH, SIR/2(26), <2007>, 10166 - 10180;
 BABS-6716975

Reaction:

RX
 Reaction ID (.ID): 10767216
 Reactant BRN (.RBRN): 11028913
 Reactant (.RCT): 9,10-dihydro-4-phenyl-9,10-<1',2'>benzeno-

10/772,445

Product BRN (.PBRN): 2,3-diazaanthracen-1(2H)-one
 11029222
 Product (.PRO): 1-chloro-9,10-dihydro-4-phenyl-9,10-<1',2'
 >benzeno-2,3-diazaanthracene
 No. of React. Details (.NVAR): 1

Reaction Details:

RX

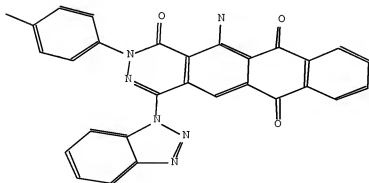
Reaction RID (.RID): 10767216.1
 Reaction Classification (.CL): Preparation
 Yield (.YDT): 90 percent (BRN=11029222)
 Reagent (.RGT): POC13
 Other Conditions (.COND): Heating
 Reference(s):

1. Bouffard, Jean; Eaton, Robert F.; Mueller, Peter; Swager, Timothy M.,
 J. Org. Chem., CODEN: JOCEAH, SIR72(26), <2007>, 10166 - 10180;
 BABS-6716975

=> d ide 139 5

L39 ANSWER 5 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN): 9968931
 Chemical Name (CN): 12-amino-4-benzotriazol-1-yl-2-p-tolyl-2H-
 2,3-diazanaphthacene-1,6,11-trione
 Autonom Name (AUN): 12-amino-4-benzotriazol-1-yl-2-p-tolyl-2H-
 2,3-diaza-naphthacene-1,6,11-trione
 Molec. Formula (MF): C29 H18 N6 O3
 Molecular Weight (MW): 498.50
 Lawson Number (LN): 30004, 29939, 16445
 Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 8391057
 Tautomer ID (TAUTID): 9323912
 Entry Date (DED): 2005/07/22
 Update Date (DUPD): 2005/07/22



Field Availability:

| Code | Name | Occurrence |
|--------|------------------------------|------------|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| AUN | Autononname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 3 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |
| CPD | Crystal Property Description | 1 |
| MP | Melting Point | 1 |
| NMR | Nuclear Magnetic Resonance | 2 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|-------|-------------------------------|------------|
| RX | Reaction Documents | 1 |
| RXPRO | Substance is Reaction Product | 1 |

=> d rx 139 5

L39 ANSWER 5 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:

```

RX
  Reaction ID (.ID):          9815714
  Reactant BRN (.RBRN):      8507609, 878524
  Reactant (.RCT):           7-amino-4-benzotriazol-1-yl-2-p-tolyl-2H-t
                             hieno<3,4-d>pyridazin-1-one,
                             <1,4>naphthoquinone
  Product BRN (.PBRN):      9968931
  Product (.PRO):           12-amino-4-benzotriazol-1-yl-2-p-tolyl-2H-
                             2,3-diaza-naphthacene-1,6,11-trione
  No. of React. Details (.NVAR): 1

```

Reaction Details:

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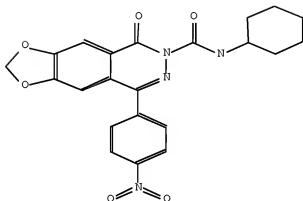
RX
  Reaction RID (.RID):       9815714.1
  Reaction Classification (.CL): Preparation
  Yield (.YDT):             56 percent (BRN=9968931)
  Solvent (.SOL):           ethanol
  Time (.TIM):              10 hour(s)
  Other Conditions (.COND): Heating
  Reference(s):
  1. Al-Saleh, Balkis; Abdelkhalik, Mervat M.; El-Asasery, Morsy A.;
     Elnagdi, Mohamed H., J. Chem. Res. Synop., CODEN: JRPSDC(1), <2005>, 23
     - 26; BABS-6487077

```

=> d ide 139 6

L39 ANSWER 6 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN): 8806911
 Chemical Name (CN): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid cyclohexylamide
 Autonom Name (AUN): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid cyclohexylamide
 Molec. Formula (MF): C22 H20 N4 O6
 Molecular Weight (MW): 436.42
 Lawson Number (LN): 32359, 14011, 1762
 Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 7455547
 Tautomer ID (TAUTID): 8275854
 Entry Date (DED): 2001/07/25
 Update Date (DUPD): 2007/02/05



Field Availability:

| Code | Name | Occurrence |
|--------|-------------------|------------|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 3 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|-------|--------------------------------|------------|
| RX | Reaction Documents | 2 |
| RXREA | Substance is Reaction Reactant | 1 |

=> d rx 139 6

L39 ANSWER 6 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:

RX

Reaction ID (.ID): 8765119
 Reactant BRN (.RBRN): 8786746, 507983
 Reactant (.RCT): 8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>p
 hthalazin-5-one, isocyanatocyclohexane
 Product BRN (.PBRN): 8806911
 Product (.PRO): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4
 ,5-g>phthalazine-6-carboxylic acid
 cyclohexylamide
 No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID): 8765119.1
 Reaction Classification (.CL): Preparation
 Reagent (.RGT): Et3N
 Solvent (.SOL): CH2Cl2
 Time (.TIM): 36 hour(s)
 Temperature (.T): 20 Cel
 Reaction Type (.TYP): Addition
 Reference(s):
 1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale,
 Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo
 De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
 BABS-6281753
 2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale,
 Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo
 De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
 BABS-6592638

Reaction:

RX

Reaction ID (.ID): 8790320
 Reactant BRN (.RBRN): 8806911
 Reactant (.RCT): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4
 ,5-g>phthalazine-6-carboxylic acid
 cyclohexylamide
 Product BRN (.PBRN): 8805983
 Product (.PRO): 8-(4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4
 ,5-g>phthalazine-6-carboxylic acid
 cyclohexylamide
 No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID): 8790320.1
 Reaction Classification (.CL): Preparation
 Yield (.YDT): 231 mg (BRN=8805983)
 Reagent (.RGT): H2
 Catalyst (.CAT): 5 percent Pd/C
 Solvent (.SOL): methanol

10/772,445

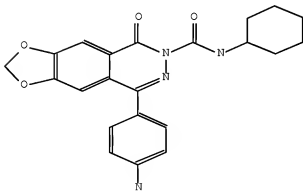
Time (.TIM): 3 hour(s)
 Temperature (.T): 20 Cel
 Reaction Type (.TYP): Catalytic hydrogenation
 Reference(s):

1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

=> d ide 139 7

L39 ANSWER 7 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

| | |
|---------------------------|--|
| Beilstein Records (BRN): | 8805983 |
| Chemical Name (CN): | 4-(4-aminophenyl)-2-cyclohexylcarbamoyl-6,7-methylenedioxypthalazin-1(2H)-one |
| Autonom Name (AUN): | 8-(4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid cyclohexylamide |
| Molec. Formula (MF): | C22 H22 N4 O4 |
| Molecular Weight (MW): | 406.44 |
| Lawson Number (LN): | 32399, 14011, 1762 |
| Compound Type (CTYPE): | heterocyclic |
| Constitution ID (CONSID): | 7454782 |
| Tautomer ID (TAUTID): | 8283445 |
| Entry Date (DED): | 2001/07/25 |
| Update Date (DUPD): | 2007/02/05 |



Field Availability:

Code Name

Occurrence

| | | |
|--------|----------------------------|---|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 3 |
| FS | File Segment | 1 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |
| MP | Melting Point | 1 |
| NMR | Nuclear Magnetic Resonance | 5 |
| PHARM | Pharmacological Data | 4 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|-------|-------------------------------|------------|
| RX | Reaction Documents | 1 |
| RXPRO | Substance is Reaction Product | 1 |

=> d rx 139 7

L39 ANSWER 7 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:

RX

| | |
|--------------------------------|---|
| Reaction ID (.ID): | 8790320 |
| Reactant BRN (.RBRN): | 8806911 |
| Reactant (.RCT): | 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid cyclohexylamide |
| Product BRN (.PBRN): | 8805983 |
| Product (.PRO): | 8-(4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid cyclohexylamide |
| No. of React. Details (.NVAR): | 1 |

Reaction Details:

RX

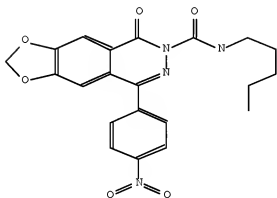
| | |
|--------------------------------|---|
| Reaction RID (.RID): | 8790320.1 |
| Reaction Classification (.CL): | Preparation |
| Yield (.YDT): | 231 mg (BRN=8805983) |
| Reagent (.RGT): | H2 |
| Catalyst (.CAT): | 5 percent Pd/C |
| Solvent (.SOL): | methanol |
| Time (.TIM): | 3 hour(s) |
| Temperature (.T): | 20 Cel |
| Reaction Type (.TYP): | Catalytic hydrogenation |
| Reference(s): | 1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753 |
| | 2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, |

Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo
 De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
 BABS-6592638

=> d ide 139 8

L39 ANSWER 8 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

| | |
|---------------------------|---|
| Beilstein Records (BRN): | 8805084 |
| Chemical Name (CN): | 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid pentylamide |
| Autonom Name (AUN): | 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid pentylamide |
| Molec. Formula (MF): | C21 H20 N4 O6 |
| Molecular Weight (MW): | 424.41 |
| Lawson Number (LN): | 32359, 2853, 1762 |
| Compound Type (CTYPE): | heterocyclic |
| Constitution ID (CONSID): | 7454058 |
| Tautomer ID (TAUTID): | 8274795 |
| Entry Date (DED): | 2001/07/25 |
| Update Date (DUPD): | 2007/02/05 |



Field Availability:

| Code | Name | Occurrence |
|--------|-------------------|------------|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 3 |
| FS | File Segment | 1 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |

| | | |
|--------|-------------|---|
| TAUTID | Tautomer ID | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|-------|--------------------------------|------------|
| RX | Reaction Documents | 2 |
| RXREA | Substance is Reaction Reactant | 1 |
| RXPRO | Substance is Reaction Product | 1 |

=> d rx 139 8

L39 ANSWER 8 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:

RX

| | |
|--------------------------------|---|
| Reaction ID (.ID): | 8748671 |
| Reactant BRN (.RBRN): | 8786746, 1746688 |
| Reactant (.RCT): | 8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>p hthalazin-5-one, pentyl isocyanate |
| Product BRN (.PBRN): | 8805084 |
| Product (.PRO): | 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4, 5-g>phthalazine-6-carboxylic acid pentylamide |
| No. of React. Details (.NVAR): | 1 |

Reaction Details:

RX

| | |
|--------------------------------|-------------|
| Reaction RID (.RID): | 8748671.1 |
| Reaction Classification (.CL): | Preparation |
| Reagent (.RGT): | Et3N |
| Solvent (.SOL): | CH2Cl2 |
| Time (.TIM): | 36 hour(s) |
| Temperature (.T): | 20 Cel |
| Reaction Type (.TYP): | Addition |
| Reference(s): | |

- Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
- Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

Reaction:

RX

| | |
|-----------------------|---|
| Reaction ID (.ID): | 8789734 |
| Reactant BRN (.RBRN): | 8805084 |
| Reactant (.RCT): | 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4, 5-g>phthalazine-6-carboxylic acid pentylamide |
| Product BRN (.PBRN): | 8802703 |
| Product (.PRO): | 8-(4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4, 5-g>phthalazine-6-carboxylic acid pentylamide |

No. of React. Details (.NVAR): 1

Reaction Details:

RX

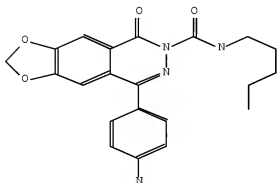
Reaction RID (.RID): 8789734.1
 Reaction Classification (.CL): Preparation
 Yield (.YDT): 255 mg (BRN=8802703)
 Reagent (.RGT): H2
 Catalyst (.CAT): 5 percent Pd/C
 Solvent (.SOL): methanol
 Time (.TIM): 3 hour(s)
 Temperature (.T): 20 Cel
 Reaction Type (.TYP): Catalytic hydrogenation
 Reference(s):

1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

=> d ide 139 9

L39 ANSWER 9 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN): 8802703
 Chemical Name (CN): 4-(4-aminophenyl)-6,7-methylenedioxy-2-pentylcarbamoylphthalazin-1(2H)-one
 Autonom Name (AUN): 8-(4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid
 pentylamide
 Molec. Formula (MF): C21 H22 N4 O4
 Molecular Weight (MW): 394.43
 Lawson Number (LN): 32399, 2853, 1762
 Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 7452174
 Tautomer ID (TAUTID): 8281628
 Entry Date (DED): 2001/07/25
 Update Date (DUPD): 2007/02/05



Field Availability:

| Code | Name | Occurrence |
|--------|----------------------------|------------|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 3 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |
| MP | Melting Point | 1 |
| MS | Mass Spectrum | 1 |
| NMR | Nuclear Magnetic Resonance | 5 |
| PHARM | Pharmacological Data | 4 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|-------|-------------------------------|------------|
| RX | Reaction Documents | 1 |
| RXPRO | Substance is Reaction Product | 1 |

=> d rx 139 9

L39 ANSWER 9 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:

RX

| | |
|--------------------------------|---|
| Reaction ID (.ID): | 8789734 |
| Reactant BRN (.RBRN): | 8805084 |
| Reactant (.RCT): | 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid pentylamide |
| Product BRN (.PBRN): | 8802703 |
| Product (.PRO): | 8-(4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid pentylamide |
| No. of React. Details (.NVAR): | 1 |

Reaction Details:

RX

| | |
|--------------------------------|----------------------|
| Reaction RID (.RID): | 8789734.1 |
| Reaction Classification (.CL): | Preparation |
| Yield (.YDT): | 255 mg (BRN=8802703) |
| Reagent (.RGT): | H2 |
| Catalyst (.CAT): | 5 percent Pd/C |
| Solvent (.SOL): | methanol |
| Time (.TIM): | 3 hour(s) |
| Temperature (.T): | 20 Cel |

Reaction Type (.TYP):

Catalytic hydrogenation

Reference(s):

1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

=> d ide 139 10

L39 ANSWER 10 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN):

8802426

Chemical Name (CN):

4-(3-aminophenyl)-2-butylcarbamoyl-6,7-methylenedioxyphthalazin-1(2H)-one

Autonom Name (AUN):

8-(3-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid
butylamide

Molec. Formula (MF):

C20 H20 N4 O4

Molecular Weight (MW):

380.40

Lawson Number (LN):

32399, 2844, 1762

Compound Type (CTYPE):

heterocyclic

Constitution ID (CONSID):

7451936

Tautomer ID (TAUTID):

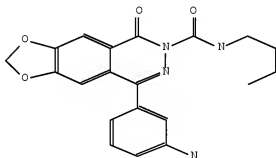
8288967

Entry Date (DED):

2001/07/25

Update Date (DUPD):

2007/02/05



Field Availability:

| Code | Name | Occurrence |
|-------|-------------------|------------|
| ===== | ===== | ===== |
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 3 |

| | | |
|--------|----------------------------|---|
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |
| MP | Melting Point | 1 |
| MS | Mass Spectrum | 1 |
| NMR | Nuclear Magnetic Resonance | 5 |
| PHARM | Pharmacological Data | 4 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|-------|-------------------------------|------------|
| RX | Reaction Documents | 1 |
| RXPRO | Substance is Reaction Product | 1 |

=> d rx 139 10

L39 ANSWER 10 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:

RX

| | |
|--------------------------------|---|
| Reaction ID (.ID): | 8788563 |
| Reactant BRN (.RBRN): | 8801393 |
| Reactant (.RCT): | 8-(3-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid butylamide |
| Product BRN (.PBRN): | 8802426 |
| Product (.PRO): | 8-(3-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid butylamide |
| No. of React. Details (.NVAR): | 1 |

Reaction Details:

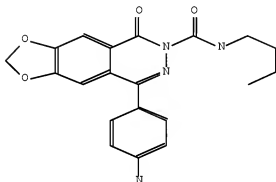
RX

| | |
|--------------------------------|---|
| Reaction RID (.RID): | 8788563.1 |
| Reaction Classification (.CL): | Preparation |
| Yield (.YDT): | 250 mg (BRN=8802426) |
| Reagent (.RG): | H2 |
| Catalyst (.CAT): | 5 percent Pd/C |
| Solvent (.SOL): | methanol |
| Time (.TIM): | 3 hour(s) |
| Temperature (.T): | 20 Cel |
| Reaction Type (.TYP): | Catalytic hydrogenation |
| Reference(s): | |
| 1. | Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753 |
| 2. | Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638 |

=> d ide 139 11

L39 ANSWER 11 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN): 8801464
 Chemical Name (CN): 4-(4-aminophenyl)-2-butylcarbamoyl-6,7-methylenedioxyphthalazin-1(2H)-one
 Autonom Name (AUN): 8-(4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid butylamide
 Molec. Formula (MF): C20 H20 N4 O4
 Molecular Weight (MW): 380.40
 Lawson Number (LN): 32399, 2844, 1762
 Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 7451143
 Tautomer ID (TAUTID): 8280453
 Entry Date (DED): 2001/07/25
 Update Date (DUPD): 2007/02/05



Field Availability:

| Code | Name | Occurrence |
|--------|----------------------------|------------|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 3 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |
| MS | Mass Spectrum | 1 |
| NMR | Nuclear Magnetic Resonance | 5 |
| PHARM | Pharmacological Data | 26 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|------|------|------------|
|------|------|------------|

```
=====
RX           Reaction Documents           1
RXPRO        Substance is Reaction Product 1
```

=> d rx 139 11

L39 ANSWER 11 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:

```
RX
  Reaction ID (.ID):      8788551
  Reactant BRN (.RBRN):  8801355
  Reactant (.RCT):       8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4
                        ,5-g>phthalazine-6-carboxylic acid
                        butylamide
  Product BRN (.PBRN):   8801464
  Product (.PRO):        8-(4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4
                        ,5-g>phthalazine-6-carboxylic acid
                        butylamide
  No. of React. Details (.NVAR): 1
```

Reaction Details:

```
RX
  Reaction RID (.RID):    8788551.1
  Reaction Classification (.CL): Preparation
  Yield (.YDT):          261 mg (BRN=8801464)
  Reagent (.RGT):        H2
  Catalyst (.CAT):       5 percent Pd/C
  Solvent (.SOL):        methanol
  Time (.TIM):           3 hour(s)
  Temperature (.T):      20 Cel
  Reaction Type (.TYP):   Catalytic hydrogenation
  Reference(s):
  1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale,
    Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo
    De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
    BABS-6281753
  2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale,
    Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo
    De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
    BABS-6592638
```

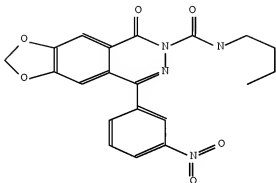
=> d ide 139 12

L39 ANSWER 12 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

```
Beilstein Records (BRN):      8801393
Chemical Name (CN):           8-(3-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4
                        ,5-g>phthalazine-6-carboxylic acid
                        butylamide
Autonom Name (AUN):          8-(3-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4
                        ,5-g>phthalazine-6-carboxylic acid
                        butylamide
Molec. Formula (MF):         C20 H18 N4 O6
Molecular Weight (MW):       410.39
Lawson Number (LN):          32359, 2844, 1762
```

10/772,445

Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 7451080
 Tautomer ID (TAUTID): 8271672
 Entry Date (DED): 2001/07/25
 Update Date (DUPD): 2007/02/05



Field Availability:

| Code | Name | Occurrence |
|--------|-------------------|------------|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 3 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|-------|--------------------------------|------------|
| RX | Reaction Documents | 2 |
| RXREA | Substance is Reaction Reactant | 1 |
| RXPRO | Substance is Reaction Product | 1 |

=> d rx 139 12

L39 ANSWER 12 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:

RX
 Reaction ID (.ID): 8774333
 Reactant BRN (.RBRN): 8787337, 773917

10/772,445

Reactant (.RCT): 8-(3-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>p
hthalazin-5-one, 1-isocyanato-butane
Product BRN (.PBRN): 8801393
Product (.PRO): 8-(3-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4
,5-g>phthalazine-6-carboxylic acid
butylamide
No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID): 8774333.1
Reaction Classification (.CL): Preparation
Reagent (.RGT): Et3N
Solvent (.SOL): CH2Cl2
Time (.TIM): 36 hour(s)
Temperature (.T): 20 Cel
Reaction Type (.TYP): Addition
Reference(s):
1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
BABS-6592638

Reaction:

RX

Reaction ID (.ID): 8788563
Reactant BRN (.RBRN): 8801393
Reactant (.RCT): 8-(3-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4
,5-g>phthalazine-6-carboxylic acid
butylamide
Product BRN (.PBRN): 8802426
Product (.PRO): 8-(3-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4
,5-g>phthalazine-6-carboxylic acid
butylamide
No. of React. Details (.NVAR): 1

Reaction Details:

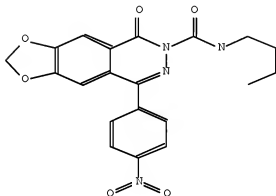
RX

Reaction RID (.RID): 8788563.1
Reaction Classification (.CL): Preparation
Yield (.YDT): 250 mg (BRN=8802426)
Reagent (.RGT): H2
Catalyst (.CAT): 5 percent Pd/C
Solvent (.SOL): methanol
Time (.TIM): 3 hour(s)
Temperature (.T): 20 Cel
Reaction Type (.TYP): Catalytic hydrogenation
Reference(s):
1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
BABS-6592638

=> d ide 139 13

L39 ANSWER 13 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN): 8801355
 Chemical Name (CN): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid butylamide
 Autonom Name (AUN): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid butylamide
 Molec. Formula (MF): C20 H18 N4 O6
 Molecular Weight (MW): 410.39
 Lawson Number (LN): 32359, 2844, 1762
 Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 7451041
 Tautomer ID (TAUTID): 8271733
 Entry Date (DED): 2001/07/25
 Update Date (DUPD): 2007/02/05



Field Availability:

| Code | Name | Occurrence |
|--------|-------------------|------------|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 3 |
| FS | File Segment | 1 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|-------|--------------------------------|------------|
| RX | Reaction Documents | 2 |
| RXREA | Substance is Reaction Reactant | 1 |
| RXPRO | Substance is Reaction Product | 1 |

=> d rx 139 13

L39 ANSWER 13 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:

RX
 Reaction ID (.ID): 8774332
 Reactant BRN (.RBRN): 8786746, 773917
 Reactant (.RCT): 8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>p
 hthalazin-5-one, 1-isocyanato-butane
 Product BRN (.PBRN): 8801355
 Product (.PRO): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,
 5-g>phthalazine-6-carboxylic acid
 butylamide
 No. of React. Details (.NVAR): 1

Reaction Details:

RX
 Reaction RID (.RID): 8774332.1
 Reaction Classification (.CL): Preparation
 Reagent (.RGT): Et3N
 Solvent (.SOL): CH2Cl2
 Time (.TIM): 36 hour(s)
 Temperature (.T): 20 Cel
 Reaction Type (.TYP): Addition
 Reference(s):
 1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale,
 Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo
 De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
 BABS-6281753
 2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale,
 Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo
 De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
 BABS-6592638

Reaction:

RX
 Reaction ID (.ID): 8788551
 Reactant BRN (.RBRN): 8801355
 Reactant (.RCT): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,
 5-g>phthalazine-6-carboxylic acid
 butylamide
 Product BRN (.PBRN): 8801464
 Product (.PRO): 8-(4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4,
 5-g>phthalazine-6-carboxylic acid
 butylamide
 No. of React. Details (.NVAR): 1

Reaction Details:

RX

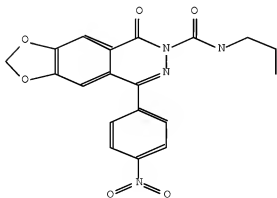
Reaction RID (.RID): 8788551.1
 Reaction Classification (.CL): Preparation
 Yield (.YDT): 261 mg (BRN=8801464)
 Reagent (.RGT): H2
 Catalyst (.CAT): 5 percent Pd/C
 Solvent (.SOL): methanol
 Time (.TIM): 3 hour(s)
 Temperature (.T): 20 Cel
 Reaction Type (.TYP): Catalytic hydrogenation
 Reference(s):

1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

=> d ide 139 14

L39 ANSWER 14 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN): 8800760
 Chemical Name (CN): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid propylamide
 Autonom Name (AUN): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid propylamide
 Molec. Formula (MF): C19 H16 N4 O6
 Molecular Weight (MW): 396.36
 Lawson Number (LN): 32359, 2835, 1762
 Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 7450482
 Tautomer ID (TAUTID): 8270366
 Entry Date (DED): 2001/07/25
 Update Date (DUPD): 2007/02/05



Field Availability:

| Code | Name | Occurrence |
|--------|-------------------|------------|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| AUN | Autononname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 3 |
| FS | File Segment | 2 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|-------|--------------------------------|------------|
| RX | Reaction Documents | 2 |
| RXREA | Substance is Reaction Reactant | 1 |
| RXPRO | Substance is Reaction Product | 1 |

=> d rx 139 14

L39 ANSWER 14 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:

RX

Reaction ID (.ID): 8741512
 Reactant BRN (.RBRN): 8786746, 1098489
 Reactant (.RCT): 8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>p
 hthalazin-5-one, 1-isocyanato-propane
 Product BRN (.PBRN): 8800760
 Product (.PRO): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4
 ,5-g>phthalazine-6-carboxylic acid
 propylamide
 No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID): 8741512.1
 Reaction Classification (.CL): Preparation
 Reagent (.RGT): Et3N
 Solvent (.SOL): CH2Cl2
 Time (.TIM): 36 hour(s)
 Temperature (.T): 20 Cel
 Reaction Type (.TYP): Addition
 Reference(s):
 1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale,
 Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo
 De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
 BABS-6281753

2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

Reaction:

RX

Reaction ID (.ID): 8788377
 Reactant BRN (.RBRN): 8800760
 Reactant (.RCT): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid
 propylamide
 Product BRN (.PBRN): 8799445
 Product (.PRO): 8-(4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid
 propylamide
 No. of React. Details (.NVAR): 1

Reaction Details:

RX

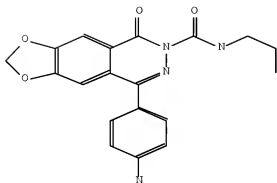
Reaction RID (.RID): 8788377.1
 Reaction Classification (.CL): Preparation
 Yield (.YDT): 268 mg (BRN=8799445)
 Reagent (.RGT): H2
 Catalyst (.CAT): 5 percent Pd/C
 Solvent (.SOL): methanol
 Time (.TIM): 3 hour(s)
 Temperature (.T): 20 Cel
 Reaction Type (.TYP): Catalytic hydrogenation
 Reference(s):

1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

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L39 ANSWER 15 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN): 8799445
 Chemical Name (CN): 4-(4-aminophenyl)-6,7-methylenedioxy-2-propylcarbamoylephthalazin-1(2H)-one
 Autonom Name (AUN): 8-(4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid
 propylamide
 Molec. Formula (MF): C19 H18 N4 O4
 Molecular Weight (MW): 366.38
 Lawson Number (LN): 32399, 2835, 1762
 Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 7449368
 Tautomer ID (TAUTID): 8279684
 Entry Date (DED): 2001/07/25
 Update Date (DUPD): 2007/02/05



Field Availability:

| Code | Name | Occurrence |
|--------|----------------------------|------------|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 3 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |
| MS | Mass Spectrum | 1 |
| NMR | Nuclear Magnetic Resonance | 5 |
| PHARM | Pharmacological Data | 4 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|-------|-------------------------------|------------|
| RX | Reaction Documents | 1 |
| RXPRO | Substance is Reaction Product | 1 |

=> d rx 139 15

L39 ANSWER 15 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:

RX

Reaction ID (.ID): 8788377
 Reactant BRN (.RBRN): 8800760
 Reactant (.RCT): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid
 propylamide
 Product BRN (.PBRN): 8799445

10/772,445

Product (.PRO): 8-(4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4
,5-g>phthalazine-6-carboxylic acid
propylamide
No. of React. Details (.NVAR): 1

Reaction Details:

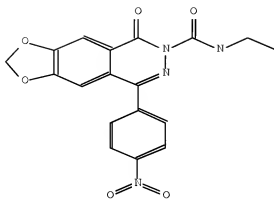
RX

Reaction RID (.RID): 8788377.1
Reaction Classification (.CL): Preparation
Yield (.YDT): 268 mg (BRN=8799445)
Reagent (.RGT): H2
Catalyst (.CAT): 5 percent Pd/C
Solvent (.SOL): methanol
Time (.TIM): 3 hour(s)
Temperature (.T): 20 Cel
Reaction Type (.TYP): Catalytic hydrogenation
Reference(s):
1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

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L39 ANSWER 16 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN): 8798692
Chemical Name (CN): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4
,5-g>phthalazine-6-carboxylic acid
ethylamide
Autonom Name (AUN): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4
,5-g>phthalazine-6-carboxylic acid
ethylamide
Molec. Formula (MF): C18 H14 N4 O6
Molecular Weight (MW): 382.33
Lawson Number (LN): 32359, 2826, 1762
Compound Type (CTYPE): heterocyclic
Constitution ID (CONSID): 7448692
Tautomer ID (TAUTID): 8270132
Entry Date (DED): 2001/07/25
Update Date (DUPD): 2007/02/05



Field Availability:

| Code | Name | Occurrence |
|--------|-------------------|------------|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 3 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|-------|--------------------------------|------------|
| RX | Reaction Documents | 2 |
| RXREA | Substance is Reaction Reactant | 1 |
| RXPRO | Substance is Reaction Product | 1 |

=> d rx 139 16

L39 ANSWER 16 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:

RX

Reaction ID (.ID): 8774240
 Reactant BRN (.RBRN): 8786746, 773743
 Reactant (.RCT): 8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>p
 hthalazin-5-one, isocyanatoethane
 Product BRN (.PBRN): 8798692
 Product (.PRO): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4
 ,5-g>phthalazine-6-carboxylic acid
 ethylamide
 No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID): 8774240.1
 Reaction Classification (.CL): Preparation
 Reagent (.RGT): Et3N
 Solvent (.SOL): CH2Cl2
 Time (.TIM): 36 hour(s)
 Temperature (.T): 20 Cel
 Reaction Type (.TYP): Addition
 Reference(s):

1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

Reaction:

RX

Reaction ID (.ID): 8787810
 Reactant BRN (.RBRN): 8798692
 Reactant (.RCT): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid ethylamide
 Product BRN (.PBRN): 8797201
 Product (.PRO): 8-(4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid ethylamide
 No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID): 8787810.1
 Reaction Classification (.CL): Preparation
 Yield (.YDI): 272 mg (BRN=8797201)
 Reagent (.RGT): H2
 Catalyst (.CAT): 5 percent Pd/C
 Solvent (.SOL): methanol
 Time (.TIM): 3 hour(s)
 Temperature (.T): 20 Cel
 Reaction Type (.TYP): Catalytic hydrogenation
 Reference(s):

1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

=> d ide 139 17

10/772,445

Beilstein Records (BRN):

Chemical Name (CN):

Autonom Name (AUN):

Molec. Formula (MF):

Molecular Weight (MW):

Lawson Number (LN):

Compound Type (CTYPE):

Constitution ID (CONSID):

Tautomer ID (TAUTID):

Entry Date (DED):

Update Date (DUPD):

8797201

4-(4-aminophenyl)-2-ethylcarbamoyl-6,7-methylenedioxyphthalazin-1(2H)-one

8-(4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid ethylamide

C18 H16 N4 O4

352.35

32399, 2826, 1762

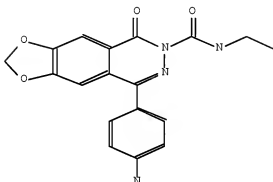
heterocyclic

7447398

8277448

2001/07/25

2007/02/05



Field Availability:

| Code | Name | Occurrence |
|--------|----------------------------|------------|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 3 |
| FS | File Segment | 2 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |
| MS | Mass Spectrum | 1 |
| NMR | Nuclear Magnetic Resonance | 5 |
| PHARM | Pharmacological Data | 4 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|------|--------------------|------------|
| RX | Reaction Documents | 1 |

=> d rx 139 17

L39 ANSWER 17 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:

RX

Reaction ID (.ID): 8787810
 Reactant BRN (.RBRN): 8798692
 Reactant (.RCT): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid ethylamide
 Product BRN (.PBRN): 8797201
 Product (.PRO): 8-(4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid ethylamide
 No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID): 8787810.1
 Reaction Classification (.CL): Preparation
 Yield (.YDT): 272 mg (BRN=8797201)
 Reagent (.RGT): H2
 Catalyst (.CAT): 5 percent Pd/C
 Solvent (.SOL): methanol
 Time (.TIM): 3 hour(s)
 Temperature (.T): 20 Cel
 Reaction Type (.TYP): Catalytic hydrogenation
 Reference(s):
 1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
 2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

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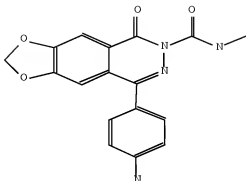
L39 ANSWER 18 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN): 8796253
 Chemical Name (CN): 4-(4-aminophenyl)-2-methylcarbamoyl-6,7-methylenedioxypthalazin-1(2H)-one
 Autonom Name (AUN): 8-(4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid methylamide
 Molec. Formula (MF): C17 H14 N4 O4
 Molecular Weight (MW): 338.32
 Lawson Number (LN): 32399, 2817, 1762
 Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 7446672
 Tautomer ID (TAUTID): 8276307

10/772,445

Entry Date (DED):
Update Date (DUPD):

2001/07/25
2007/02/05



Field Availability:

| Code | Name | Occurrence |
|--------|----------------------------|------------|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 3 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |
| MS | Mass Spectrum | 1 |
| NMR | Nuclear Magnetic Resonance | 5 |
| PHARM | Pharmacological Data | 4 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|-------|-------------------------------|------------|
| RX | Reaction Documents | 1 |
| RXPRO | Substance is Reaction Product | 1 |

=> d rx 139 18

L39 ANSWER 18 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:

RX

Reaction ID (.ID): 8787000
 Reactant BRN (.RBRN): 8795870
 Reactant (.RCT): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4

10/772,445

Product BRN (.PBRN): 8- (4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4
methylamide
Product (.PRO): 8- (4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4
methylamide
No. of React. Details (.NVAR): 1

Reaction Details:

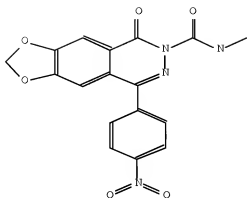
RX

Reaction RID (.RID): 8787000.1
Reaction Classification (.CL): Preparation
Yield (.YDT): 239 mg (BRN=8796253)
Reagent (.RGT): H2
Catalyst (.CAT): 5 percent Pd/C
Solvent (.SOL): methanol
Time (.TIM): 3 hour(s)
Temperature (.T): 20 Cel
Reaction Type (.TYP): Catalytic hydrogenation
Reference(s):
1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

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L39 ANSWER 19 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN): 8795870
Chemical Name (CN): 8- (4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4
methylamide
Autonom Name (AUN): 8- (4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4
methylamide
Molec. Formula (MF): C17 H12 N4 O6
Molecular Weight (MW): 368.31
Lawson Number (LN): 32359, 2817, 1762
Compound Type (CTYPE): heterocyclic
Constitution ID (CONSID): 7446283
Tautomer ID (TAUTID): 8266541
Entry Date (DED): 2001/07/25
Update Date (DUPD): 2007/02/05



Field Availability:

| Code | Name | Occurrence |
|--------|-------------------|------------|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 3 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|-------|--------------------------------|------------|
| RX | Reaction Documents | 2 |
| RXREA | Substance is Reaction Reactant | 1 |
| RXPRO | Substance is Reaction Product | 1 |

=> d rx 139 19

L39 ANSWER 19 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:

RX

Reaction ID (.ID): 8767356
 Reactant BRN (.RBRN): 8786746, 605318
 Reactant (.RCT): 8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>p
 thalazin-5-one, isocyanatomethane
 Product BRN (.PBRN): 8795870
 Product (.PRO): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4
 ,5-g>phthalazine-6-carboxylic acid
 methylamide
 No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID): 8767356.1
 Reaction Classification (.CL): Preparation
 Reagent (.RGT): Et3N
 Solvent (.SOL): CH2Cl2
 Time (.TIM): 36 hour(s)
 Temperature (.T): 20 Cel
 Reaction Type (.TYP): Addition
 Reference(s):

1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

Reaction:

RX

Reaction ID (.ID): 8787000
 Reactant BRN (.RBRN): 8795870
 Reactant (.RCT): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid methylamide
 Product BRN (.PBRN): 8796253
 Product (.PRO): 8-(4-amino-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid methylamide
 No. of React. Details (.NVAR): 1

Reaction Details:

RX

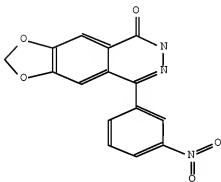
Reaction RID (.RID): 8787000.1
 Reaction Classification (.CL): Preparation
 Yield (.YDI): 239 mg (BRN=8796253)
 Reagent (.RGT): H2
 Catalyst (.CAT): 5 percent Pd/C
 Solvent (.SOL): methanol
 Time (.TIM): 3 hour(s)
 Temperature (.T): 20 Cel
 Reaction Type (.TYP): Catalytic hydrogenation
 Reference(s):

1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

=> d ide 139 20

10/772,445

Beilstein Records (BRN): 8787337
 Chemical Name (CN): 6,7-methylenedioxy-4-(3-nitrophenyl)-phthalazin-1(2H)-one
 Autonom Name (AUN): 8-(3-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>phtalazin-5-one
 Molec. Formula (MF): C15 H9 N3 O5
 Molecular Weight (MW): 311.25
 Lawson Number (LN): 32359
 Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 7439055
 Tautomer ID (TAUTID): 8280617
 Entry Date (DED): 2001/07/25
 Update Date (DUPD): 2007/02/05



Field Availability:

| Code | Name | Occurrence |
|--------|----------------------------|------------|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 1 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |
| NMR | Nuclear Magnetic Resonance | 5 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|-------|--------------------------------|------------|
| RX | Reaction Documents | 3 |
| RXREA | Substance is Reaction Reactant | 2 |
| RXPRO | Substance is Reaction Product | 1 |

=> d rx 139 20

L39 ANSWER 20 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:

RX

Reaction ID (.ID): 8782108
 Reactant BRN (.RBRN): 8778660
 Reactant (.RCT): (6-methyl-benzo<1,3>dioxol-5-yl)-(3-nitro-phenyl)-methanone
 Product BRN (.PBRN): 8787337
 Product (.PRO): 8-(3-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>p
 hthalazin-5-one
 No. of React. Details (.NVAR): 2

Reaction Details:

RX

Reaction RID (.RID): 8782108.1
 Reaction Classification (.CL): Multistage
 Yield (.YDT): 52 percent (BRN=8787337)
 Nr. of Stages (.SNR): 2
 Stage 1
 Reagent (.RGT): bromine
 Solvent (.SOL): CC14
 Time (.TIM): 8 hour(s)
 Other Conditions (.COND): Heating, UV-irradiation
 Reaction Type (.TYP): Bromination
 Stage 2
 Reagent (.RGT): NH2NH2*H2O
 Solvent (.SOL): ethanol
 Temperature (.T): 16 Cel
 Other Conditions (.COND): Heating
 Reaction Type (.TYP): Oxidation, cyclocondensation
 Reference(s):
 1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

RX

Reaction RID (.RID): 8782108.2
 Reaction Classification (.CL): Multistage
 Yield (.YDT): 52 percent (BRN=8787337)
 Nr. of Stages (.SNR): 2
 Stage 1
 Reagent (.RGT): bromine
 Solvent (.SOL): CC14
 Time (.TIM): 8 hour(s)
 Other Conditions (.COND): Heating, UV-irradiation
 Reaction Type (.TYP): Bromination, Oxidation
 Stage 2
 Reagent (.RGT): NH2NH2*H2O
 Solvent (.SOL): ethanol
 Temperature (.T): 16 Cel
 Other Conditions (.COND): Heating
 Reaction Type (.TYP): cyclocondensation
 Reference(s):
 1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale,

Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo
 De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
 BABS-6281753

Reaction:

RX
 Reaction ID (.ID): 8784730
 Reactant BRN (.RBRN): 8787337
 Reactant (.RCT): 8-(3-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>p
 hthalazin-5-one
 Product BRN (.PBRN): 8786723
 Product (.PRO): 8-(3-amino-phenyl)-6H-<1,3>dioxolo<4,5-g>p
 hthalazin-5-one
 No. of React. Details (.NVAR): 1

Reaction Details:

RX
 Reaction RID (.RID): 8784730.1
 Reaction Classification (.CL): Preparation
 Yield (.YDT): 87 percent (BRN=8786723)
 Reagent (.RGT): H2
 Catalyst (.CAT): 5 percent Pd/C
 Solvent (.SOL): methanol
 Time (.TIM): 3 hour(s)
 Temperature (.T): 20 Cel
 Reaction Type (.TYP): Catalytic hydrogenation
 Reference(s):
 1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale,
 Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo
 De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
 BABS-6281753
 2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale,
 Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo
 De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
 BABS-6592638

Reaction:

RX
 Reaction ID (.ID): 8774333
 Reactant BRN (.RBRN): 8787337, 773917
 Reactant (.RCT): 8-(3-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>p
 hthalazin-5-one, 1-isocyanato-butane
 Product BRN (.PBRN): 8801393
 Product (.PRO): 8-(3-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,
 5-g>phthalazine-6-carboxylic acid
 butylamide
 No. of React. Details (.NVAR): 1

Reaction Details:

RX
 Reaction RID (.RID): 8774333.1
 Reaction Classification (.CL): Preparation
 Reagent (.RGT): Et3N
 Solvent (.SOL): CH2Cl2
 Time (.TIM): 36 hour(s)
 Temperature (.T): 20 Cel
 Reaction Type (.TYP): Addition
 Reference(s):
 1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale,
 Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo

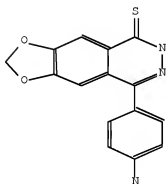
De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
BABS-6281753

2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo
De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
BABS-6592638

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L39 ANSWER 21 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

| | |
|---------------------------|--|
| Beilstein Records (BRN): | 8786898 |
| Chemical Name (CN): | 4-(4-aminophenyl)-6,7-methylenedioxyphthalazine-1(2H)-thione |
| Autonom Name (AUN): | 8-(4-amino-phenyl)-6H-<1,3>dioxolo<4,5-g>phtalazine-5-thione |
| Molec. Formula (MF): | C15 H11 N3 O2 S |
| Molecular Weight (MW): | 297.33 |
| Lawson Number (LN): | 32394 |
| Compound Type (CTYPE): | heterocyclic |
| Constitution ID (CONSID): | 7438673 |
| Tautomer ID (TAUTID): | 8279184 |
| Entry Date (DED): | 2001/07/25 |
| Update Date (DUPD): | 2007/02/05 |



Field Availability:

| Code | Name | Occurrence |
|-------|-------------------|------------|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 1 |
| CTYPE | Compound Type | 1 |

| | | |
|--------|----------------------------|---|
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |
| NMR | Nuclear Magnetic Resonance | 5 |
| PHARM | Pharmacological Data | 4 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|-------|-------------------------------|------------|
| RX | Reaction Documents | 1 |
| RXPRO | Substance is Reaction Product | 1 |

=> d rx 139 21

L39 ANSWER 21 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:

RX

| | |
|--------------------------------|--|
| Reaction ID (.ID): | 8784559 |
| Reactant BRN (.RBRN): | 8786694 |
| Reactant (.RCT): | 8-(4-amino-phenyl)-6H-<1,3>dioxolo<4,5-g>p ththalazin-5-one |
| Product BRN (.PBRN): | 8786898 |
| Product (.PRO): | 8-(4-amino-phenyl)-6H-<1,3>dioxolo<4,5-g>p ththalazine-5-thione |
| No. of React. Details (.NVAR): | 1 |

Reaction Details:

RX

| | |
|--------------------------------|--------------------------|
| Reaction RID (.RID): | 8784559.1 |
| Reaction Classification (.CL): | Preparation |
| Yield (.YDT): | 82 percent (BRN=8786898) |
| Reagent (.RGT): | Lawesson's reagent |
| Solvent (.SOL): | toluene |
| Time (.TIM): | 2 hour(s) |
| Other Conditions (.COND): | Heating |
| Reaction Type (.TYP): | Substitution |

Reference(s):

1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

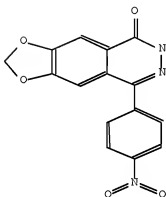
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L39 ANSWER 22 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

| | |
|--------------------------|---|
| Beilstein Records (BRN): | 8786746 |
| Chemical Name (CN): | 6,7-methylenedioxy-4-(4-nitrophenyl)-phthalazin-1(2H)-one |

10/772,445

Autonom Name (AUN): 8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>p
 hthalazin-5-one
 Molec. Formula (MF): C15 H9 N3 O5
 Molecular Weight (MW): 311.25
 Lawson Number (LN): 32359
 Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 7438558
 Tautomer ID (TAUTID): 8281644
 Entry Date (DED): 2001/07/25
 Update Date (DUPD): 2007/02/05



Field Availability:

| Code | Name | Occurrence |
|--------|----------------------------|------------|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 1 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |
| MP | Melting Point | 1 |
| NMR | Nuclear Magnetic Resonance | 5 |
| PHARM | Pharmacological Data | 1 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|-------|--------------------------------|------------|
| RX | Reaction Documents | 10 |
| RXREA | Substance is Reaction Reactant | 8 |
| RXPRO | Substance is Reaction Product | 2 |

=> d rx 139 22

L39 ANSWER 22 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:

RX

Reaction ID (.ID): 9460950
 Reactant BRN (.RBRN): 331047
 Reactant (.RCT): 6-(4-nitro-benzoyl)-benzo<1,3>dioxole-5-carboxylic acid
 8786746
 Product BRN (.PBRN):
 Product (.PRO): 8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>pythalazin-5-one
 No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID): 9460950.1
 Reaction Classification (.CL): Preparation
 Reagent (.RGT): aq. H2NNH2
 Solvent (.SOL): ethanol
 Other Conditions (.COND): Heating
 Reference(s):
 1. Solyom, Sandor; Hamori, Tamas; Borosy, Andras P.; Tarnawa, Istvan; Bersenyi, Pal; Pallagi, Istvan, Med.Chem.Res., CODEN: MCREEB, 11(1), <2002>, 39 - 49; BABS-6420582

Reaction:

RX

Reaction ID (.ID): 8782107
 Reactant BRN (.RBRN): 8778659
 Reactant (.RCT): (6-methyl-benzo<1,3>dioxol-5-yl)-(4-nitro-phenyl)-methanone
 8786746
 Product BRN (.PBRN):
 Product (.PRO): 8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>pythalazin-5-one
 No. of React. Details (.NVAR): 2

Reaction Details:

RX

Reaction RID (.RID): 8782107.1
 Reaction Classification (.CL): Multistage
 Yield (.YDT): 55 percent (BRN=8786746)
 Nr. of Stages (.SNR): 2
 Stage 1
 Reagent (.RGT): bromine
 Solvent (.SOL): CCl4
 Time (.TIM): 8 hour(s)
 Other Conditions (.COND): Heating, UV-irradiation
 Reaction Type (.TYP): Bromination
 Stage 2
 Reagent (.RGT): NH2NH2*H2O
 Solvent (.SOL): ethanol
 Temperature (.T): 16 Cel
 Other Conditions (.COND): Heating
 Reaction Type (.TYP): Oxidation, cyclocondensation
 Reference(s):

1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
BABS-6592638

RX

Reaction RID (.RID): 8782107.2
 Reaction Classification (.CL): Multistage
 Yield (.YDT): 55 percent (BRN=8786746)
 Nr. of Stages (.SNR): 2
 Stage 1
 Reagent (.RGT): bromine
 Solvent (.SOL): CCl4
 Time (.TIM): 8 hour(s)
 Other Conditions (.COND): Heating, UV-irradiation
 Reaction Type (.TYP): Bromination, Oxidation
 Stage 2
 Reagent (.RGT): NH2NH2*H2O
 Solvent (.SOL): ethanol
 Temperature (.T): 16 Cel
 Other Conditions (.COND): Heating
 Reaction Type (.TYP): cyclocondensation
 Reference(s):
 1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
BABS-6281753

Reaction:

RX

Reaction ID (.ID): 9481786
 Reactant BRN (.RBRN): 8786746
 Reactant (.RCT): 8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>p
 hthalazin-5-one
 Product BRN (.PBRN): 9575008
 Product (.PRO): 5-chloro-8-(4-nitro-phenyl)-<1,3>dioxolo<4
 ,5-g>phthalazine
 No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID): 9481786.1
 Reaction Classification (.CL): Preparation
 Reagent (.RGT): POC13
 Other Conditions (.COND): Heating
 Reference(s):
 1. Solyom, Sandor; Hamori, Tamas; Borosy, Andras P.; Tarnawa, Istvan; Bersenyi, Pal; Pallagi, Istvan, Med. Chem. Res., CODEN: MCREEB, 11(1), <2002>, 39 - 49; BABS-6420582

Reaction:

RX

Reaction ID (.ID): 8784574
 Reactant BRN (.RBRN): 8786746
 Reactant (.RCT): 8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>p
 hthalazin-5-one
 Product BRN (.PBRN): 8786694
 Product (.PRO): 8-(4-amino-phenyl)-6H-<1,3>dioxolo<4,5-g>p
 hthalazin-5-one
 No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID): 8784574.1
 Reaction Classification (.CL): Preparation
 Yield (.YDT): 89 percent (BRN=8786694)
 Reagent (.RGT): H₂
 Catalyst (.CAT): 5 percent Pd/C
 Solvent (.SOL): methanol
 Time (.TIM): 3 hour(s)
 Temperature (.T): 20 Cel
 Reaction Type (.TYP): Catalytic hydrogenation
 Reference(s):
 1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
 2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

Reaction:

RX

Reaction ID (.ID): 8774332
 Reactant BRN (.RBRN): 8786746, 773917
 Reactant (.RCT): 8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>p
 hthalazin-5-one, 1-isocyanato-butane
 8801355
 Product BRN (.PBRN):
 Product (.PRO): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4
 ,5-g>phthalazine-6-carboxylic acid
 butylamide
 No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID): 8774332.1
 Reaction Classification (.CL): Preparation
 Reagent (.RGT): Et₃N
 Solvent (.SOL): CH₂Cl₂
 Time (.TIM): 36 hour(s)
 Temperature (.T): 20 Cel
 Reaction Type (.TYP): Addition
 Reference(s):
 1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
 2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

Reaction:

RX

Reaction ID (.ID): 8774240
 Reactant BRN (.RBRN): 8786746, 773743
 Reactant (.RCT): 8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>p
 hthalazin-5-one, isocyanatoethane
 8798692
 Product BRN (.PBRN):
 Product (.PRO): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4

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,5-g>phthalazine-6-carboxylic acid
ethylamide

No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID): 8774240.1
 Reaction Classification (.CL): Preparation
 Reagent (.RGT): Et3N
 Solvent (.SOL): CH2Cl2
 Time (.TIM): 36 hour(s)
 Temperature (.T): 20 Cel
 Reaction Type (.TYP): Addition

Reference(s):

1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
BABS-6592638

Reaction:

RX

Reaction ID (.ID): 8767356
 Reactant BRN (.RBRN): 8786746, 605318
 Reactant (.RCT): 8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>p
hthalazin-5-one, isocyanatomethane
 Product BRN (.PBRN): 8795870
 Product (.PRO): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4
,5-g>phthalazine-6-carboxylic acid
methylamide

No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID): 8767356.1
 Reaction Classification (.CL): Preparation
 Reagent (.RGT): Et3N
 Solvent (.SOL): CH2Cl2
 Time (.TIM): 36 hour(s)
 Temperature (.T): 20 Cel
 Reaction Type (.TYP): Addition

Reference(s):

1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
BABS-6592638

Reaction:

RX

Reaction ID (.ID): 8765119
 Reactant BRN (.RBRN): 8786746, 507983
 Reactant (.RCT): 8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>p
hthalazin-5-one, isocyanatocyclohexane

10/772,445

Product BRN (.PBRN): 8806911
 Product (.PRO): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid
 cyclohexylamide
 No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID): 8765119.1
 Reaction Classification (.CL): Preparation
 Reagent (.RGT): Et3N
 Solvent (.SOL): CH2Cl2
 Time (.TIM): 36 hour(s)
 Temperature (.T): 20 Cel
 Reaction Type (.TYP): Addition
 Reference(s):

1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
 BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
 BABS-6592638

Reaction:

RX

Reaction ID (.ID): 8748671
 Reactant BRN (.RBRN): 8786746, 1746688
 Reactant (.RCT): 8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>p
 hthalazin-5-one, pentyl isocyanate
 Product BRN (.PBRN): 8805084
 Product (.PRO): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4,5-g>phthalazine-6-carboxylic acid
 pentylamide
 No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID): 8748671.1
 Reaction Classification (.CL): Preparation
 Reagent (.RGT): Et3N
 Solvent (.SOL): CH2Cl2
 Time (.TIM): 36 hour(s)
 Temperature (.T): 20 Cel
 Reaction Type (.TYP): Addition
 Reference(s):

1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
 BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
 BABS-6592638

Reaction:

RX

Reaction ID (.ID): 8741512
 Reactant BRN (.RBRN): 8786746, 1098489

10/772,445

Reactant (.RCT): 8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>p
hthalazin-5-one, 1-isocyanato-propane
Product BRN (.PBRN): 8800760
Product (.PRO): 8-(4-nitro-phenyl)-5-oxo-5H-<1,3>dioxolo<4
,5-g>phthalazine-6-carboxylic acid
propylamide
No. of React. Details (.NVAR): 1

Reaction Details:

RX

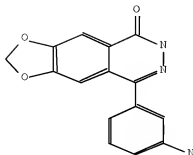
Reaction RID (.RID): 8741512.1
Reaction Classification (.CL): Preparation
Reagent (.RGT): Et3N
Solvent (.SOL): CH2Cl2
Time (.TIM): 36 hour(s)
Temperature (.T): 20 Cel
Reaction Type (.TYP): Addition
Reference(s):

1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

=> d ide 139 23

L39 ANSWER 23 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN): 8786723
Chemical Name (CN): 4-(3-aminophenyl)-6,7-methylenedioxyphthal
azin-1(2H)-one
Autonom Name (AUN): 8-(3-amino-phenyl)-6H-<1,3>dioxolo<4,5-g>p
hthalazin-5-one
Molec. Formula (MF): C15 H11 N3 O3
Molecular Weight (MW): 281.27
Lawson Number (LN): 32399
Compound Type (CTYPE): heterocyclic
Constitution ID (CONSID): 7438541
Tautomer ID (TAUTID): 8278845
Entry Date (DED): 2001/07/25
Update Date (DUPD): 2007/02/05



Field Availability:

| Code | Name | Occurrence |
|--------|----------------------------|------------|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 1 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |
| MS | Mass Spectrum | 1 |
| NMR | Nuclear Magnetic Resonance | 5 |
| PHARM | Pharmacological Data | 4 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|-------|-------------------------------|------------|
| RX | Reaction Documents | 1 |
| RXPRO | Substance is Reaction Product | 1 |

=> d rx 139 23

L39 ANSWER 23 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:

RX

```

Reaction ID (.ID):      8784730
Reactant BRN (.RBRN):  8787337
Reactant (.RCT):       8-(3-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>p
                        hthalazin-5-one
Product BRN (.PBRN):   8786723
Product (.PRO):        8-(3-amino-phenyl)-6H-<1,3>dioxolo<4,5-g>p
                        hthalazin-5-one
No. of React. Details (.NVAR): 1

```

Reaction Details:

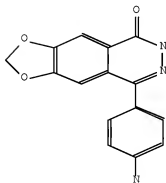
RX

Reaction RID (.RID): 8784730.1
 Reaction Classification (.CL): Preparation
 Yield (.YDT): 87 percent (BRN=8786723)
 Reagent (.RGT): H2
 Catalyst (.CAT): 5 percent Pd/C
 Solvent (.SOL): methanol
 Time (.TIM): 3 hour(s)
 Temperature (.T): 20 Cel
 Reaction Type (.TYP): Catalytic hydrogenation
 Reference(s):
 1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
 2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

=> d ide 139 24

L39 ANSWER 24 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN): 8786694
 Chemical Name (CN): 4-(4-aminophenyl)-6,7-methylenedioxyphthalazin-1(2H)-one
 Autonom Name (AUN): 8-(4-amino-phenyl)-6H-<1,3>dioxolo<4,5-g>p hthalazin-5-one
 Molec. Formula (MF): C15 H11 N3 O3
 Molecular Weight (MW): 281.27
 Lawson Number (LN): 32399
 Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 7438516
 Tautomer ID (TAUTID): 8278888
 Entry Date (DED): 2001/07/25
 Update Date (DUPD): 2007/02/05



Field Availability:

| Code | Name | Occurrence |
|--------|----------------------------|------------|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 1 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |
| NMR | Nuclear Magnetic Resonance | 5 |
| PHARM | Pharmacological Data | 28 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|-------|--------------------------------|------------|
| RX | Reaction Documents | 2 |
| RXREA | Substance is Reaction Reactant | 1 |
| RXPRO | Substance is Reaction Product | 1 |

=> d rx 139 24

L39 ANSWER 24 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:

RX

Reaction ID (.ID): 8784574
 Reactant BRN (.RBRN): 8786746
 Reactant (.RCT): 8-(4-nitro-phenyl)-6H-<1,3>dioxolo<4,5-g>p
 hthalazin-5-one
 Product BRN (.PBRN): 8786694
 Product (.PRO): 8-(4-amino-phenyl)-6H-<1,3>dioxolo<4,5-g>p
 hthalazin-5-one
 No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID): 8784574.1
 Reaction Classification (.CL): Preparation
 Yield (.YDT): 89 percent (BRN=8786694)
 Reagent (.RGT): H2
 Catalyst (.CAT): 5 percent Pd/C
 Solvent (.SOL): methanol
 Time (.TIM): 3 hour(s)
 Temperature (.T): 20 Cel
 Reaction Type (.TYP): Catalytic hydrogenation
 Reference(s):

1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;

BABS-6281753

2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
BABS-6592638

Reaction:

RX

| | |
|--------------------------------|---|
| Reaction ID (.ID): | 8784559 |
| Reactant BRN (.RBRN): | 8786694 |
| Reactant (.RCT): | 8-(4-amino-phenyl)-6H-<1,3>dioxolo<4,5-g>p hthalazin-5-one |
| Product BRN (.PBRN): | 8786898 |
| Product (.PRO): | 8-(4-amino-phenyl)-6H-<1,3>dioxolo<4,5-g>p hthalazine-5-thione |
| No. of React. Details (.NVAR): | 1 |

Reaction Details:

RX

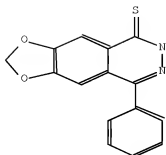
| | |
|--------------------------------|--------------------------|
| Reaction RID (.RID): | 8784559.1 |
| Reaction Classification (.CL): | Preparation |
| Yield (.YDT): | 82 percent (BRN=8786898) |
| Reagent (.RGT): | Lawesson's reagent |
| Solvent (.SOL): | toluene |
| Time (.TIM): | 2 hour(s) |
| Other Conditions (.COND): | Heating |
| Reaction Type (.TYP): | Substitution |
| Reference(s): | |

1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
BABS-6592638

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L39 ANSWER 25 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

| | |
|---------------------------|---|
| Beilstein Records (BRN): | 8780260 |
| Chemical Name (CN): | 6,7-methylenedioxy-4-phenylphthalazine-1(2 H)-thione |
| Autonom Name (AUN): | 8-phenyl-6H-<1,3>dioxolo<4,5-g>phthalazine -5-thione |
| Molec. Formula (MF): | C15 H10 N2 O2 S |
| Molecular Weight (MW): | 282.32 |
| Lawson Number (LN): | 32353 |
| Compound Type (CTYPE): | heterocyclic |
| Constitution ID (CONSID): | 7432908 |
| Tautomer ID (TAUTID): | 8277944 |
| Entry Date (DED): | 2001/07/25 |
| Update Date (DUPD): | 2007/02/05 |



Field Availability:

| Code | Name | Occurrence |
|--------|----------------------------|------------|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomous Name | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 1 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |
| MS | Mass Spectrum | 1 |
| NMR | Nuclear Magnetic Resonance | 4 |
| PHARM | Pharmacological Data | 4 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|-------|-------------------------------|------------|
| RX | Reaction Documents | 1 |
| RXPRO | Substance is Reaction Product | 1 |

=> d rx 139 25

L39 ANSWER 25 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:

RX

Reaction ID (.ID): 8782500
 Reactant BRN (.RBRN): 8780129
 Reactant (.RCT): 8-phenyl-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one
 Product BRN (.PBRN): 8780260
 Product (.PRO): 8-phenyl-6H-<1,3>dioxolo<4,5-g>phthalazine-5-thione
 No. of React. Details (.NVAR): 1

Reaction Details:

RX

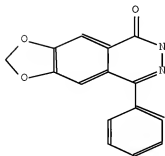
Reaction RID (.RID): 8782500.1
 Reaction Classification (.CL): Preparation
 Yield (.YDT): 85 percent (BRN=8780260)
 Reagent (.RGT): Lawesson's reagent
 Solvent (.SOL): toluene
 Time (.TIM): 2 hour(s)
 Other Conditions (.COND): Heating
 Reaction Type (.TYP): Substitution
 Reference(s):

1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J.Med.Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6281753
2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859; BABS-6592638

=> d ide 139 26

L39 ANSWER 26 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN): 8780129
 Chemical Name (CN): 6,7-methylenedioxy-4-phenylphthalazin-1(2H)-one
 Autonom Name (AUN): 8-phenyl-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one
 Molec. Formula (MF): C15 H10 N2 O3
 Molecular Weight (MW): 266.26
 Lawson Number (LN): 32358
 Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 7432813
 Tautomer ID (TAUTID): 8277953
 Entry Date (DED): 2001/07/25
 Update Date (DUPD): 2007/02/05



Field Availability:

| Code | Name | Occurrence |
|--------|----------------------------|------------|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 1 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |
| MS | Mass Spectrum | 1 |
| NMR | Nuclear Magnetic Resonance | 4 |
| PHARM | Pharmacological Data | 4 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|-------|--------------------------------|------------|
| RX | Reaction Documents | 2 |
| RXREA | Substance is Reaction Reactant | 1 |
| RXPRO | Substance is Reaction Product | 1 |

=> d rx 139 26

L39 ANSWER 26 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:

```

RX
  Reaction ID (.ID):      8766058
  Reactant BRN (.RBRN):  5544914
  Reactant (.RCT):       6-methylbenzo-1,3-dioxol-5-yl phenyl
                           ketone
  Product BRN (.PBRN):   8780129
  Product (.PRO):        8-phenyl-6H-<1,3>dioxolo<4,5-g>phthalazin-
                           5-one
  No. of React. Details (.NVAR): 2

```

Reaction Details:

```

RX
  Reaction RID (.RID):    8766058.1
  Reaction Classification (.CL): Multistage
  Yield (.YDT):          59 percent (BRN=8780129)
  Nr. of Stages (.SNR):   2
  Stage 1
  Reagent (.RGT):        bromine
  Solvent (.SOL):        CCl4
  Time (.TIM):           8 hour(s)
  Other Conditions (.COND): Heating, UV-irradiation
  Reaction Type (.TYP):   Bromination
  Stage 2
  Reagent (.RGT):        NH2NH2*H2O
  Solvent (.SOL):        ethanol
  Temperature (.T):      16 Cel

```

Other Conditions (.COND): Heating
 Reaction Type (.TYP): Oxidation, cyclocondensation
 Reference(s):
 1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
 BABS-6592638

RX

Reaction RID (.RID): 8766058.2
 Reaction Classification (.CL): Multistage
 Yield (.YDT): 59 percent (BRN=8780129)
 Nr. of Stages (.SNR): 2
 Stage 1
 Reagent (.RGT): bromine
 Solvent (.SOL): CC14
 Time (.TIM): 8 hour(s)
 Other Conditions (.COND): Heating, UV-irradiation
 Reaction Type (.TYP): Bromination, Oxidation
 Stage 2
 Reagent (.RGT): NH2NH2*H2O
 Solvent (.SOL): ethanol
 Temperature (.T): 16 Cel
 Other Conditions (.COND): Heating
 Reaction Type (.TYP): cyclocondensation
 Reference(s):
 1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
 BABS-6281753

Reaction:

RX

Reaction ID (.ID): 8782500
 Reactant BRN (.RBRN): 8780129
 Reactant (.RCT): 8-phenyl-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one
 Product BRN (.PBRN): 8780260
 Product (.PRO): 8-phenyl-6H-<1,3>dioxolo<4,5-g>phthalazine-5-thione
 No. of React. Details (.NVAR): 1

Reaction Details:

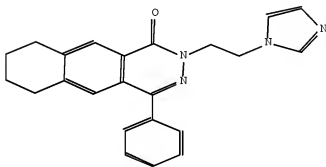
RX

Reaction RID (.RID): 8782500.1
 Reaction Classification (.CL): Preparation
 Yield (.YDT): 85 percent (BRN=8780260)
 Reagent (.RGT): Lawesson's reagent
 Solvent (.SOL): toluene
 Time (.TIM): 2 hour(s)
 Other Conditions (.COND): Heating
 Reaction Type (.TYP): Substitution
 Reference(s):
 1. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
 BABS-6281753
 2. Grasso, Silvana; Sarro, Giovambattista De; Sarro, Angela De; Micale, Nicola; Zappala, Maria; Puja, Giulia; Baraldi, Mario; Micheli, Carlo De, J. Med. Chem., CODEN: JMCMAR, 43(15), <2000>, 2851 - 2859;
 BABS-6592638

=> d ide 139 27

L39 ANSWER 27 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN): 8444536
 Chemical Name (CN): 6,7,8,9-tetrahydro-2-<2-(1-imidazolyl)ethyl
 1>-4-phenyl-benzo<g>phthalazin-1(2H)-one
 Autonom Name (AUN): 2-(2-imidazol-1-yl-ethyl)-4-phenyl-6,7,8,9
 -tetrahydro-2H-benzo<g>phthalazin-1-one
 Molec. Formula (MF): C23 H22 N4 O
 Molecular Weight (MW): 370.45
 Lawson Number (LN): 28745, 28020, 3706
 Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 7164599
 Tautomer ID (TAUTID): 7965180
 Entry Date (DED): 2000/05/16
 Update Date (DUPD): 2000/05/16



Field Availability:

| Code | Name | Occurrence |
|--------|----------------------------|------------|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 3 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |
| IR | Infrared Spectrum | 1 |
| MP | Melting Point | 1 |
| NMR | Nuclear Magnetic Resonance | 2 |

PHARM Pharmacological Data

1

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|-------|-------------------------------|------------|
| RX | Reaction Documents | 1 |
| RXPRO | Substance is Reaction Product | 1 |

=> d rx 139 27

L39 ANSWER 27 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:

RX

Reaction ID (.ID): 8533023
 Reactant BRN (.RBRN): 7434131, 4291410
 Reactant (.RCT): 6,7,8,9-tetrahydro-4-phenylbenzo<g>phthalazin-1(2H)-one,
 1-(2-chloro-ethyl)-1H-imidazole
 Product BRN (.PBRN): 8444536
 Product (.PRO): 2-(2-imidazol-1-yl-ethyl)-4-phenyl-6,7,8,9-tetrahydro-2H-benzo<g>phthalazin-1-one
 No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID): 8533023.1
 Reaction Classification (.CL): Multistage
 Yield (.YDT): 70 percent (BRN=8444536)
 Nr. of Stages (.SNR): 2
 Stage 1
 Reagent (.RGT): NaH
 Solvent (.SOL): dimethylformamide
 Time (.TIM): 1 hour(s)
 Temperature (.T): 20 Cel
 Reaction Type (.TYP): deprotonation
 Stage 2
 Stage reactant (.SRCT): 1-(2-chloro-ethyl)-1H-imidazole
 Stage Reactant BRN (.SRBRN): 4291410
 Solvent (.SOL): dimethylformamide
 Time (.TIM): 14 hour(s)
 Temperature (.T): 70 Cel
 Reaction Type (.TYP): Substitution
 Reference(s):
 1. Haider, Norbert; Hartmann, Rolf W.; Steinwender, Andreas,
 Arch.Pharm.(Weinheim Ger.), CODEN: ARPMAS, 332(11), <1999>, 408 - 409;
 BABS-6205172

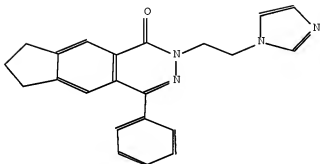
=> d ide 139 28

L39 ANSWER 28 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN): 8441980
 Chemical Name (CN): 2,6,7,8-tetrahydro-2-<2-(1-imidazolyl)ethyl
 1>-4-phenyl-1H-cyclopenta<g>phthalazin-1-one

10/772,445

ne
 6-(2-imidazol-1-yl-ethyl)-8-phenyl-1,2,3,6
 -tetrahydro-6,7-diaza-cyclopentanaphtha
 len-5-one
 Molec. Formula (MF): C22 H20 N4 O
 Molecular Weight (MW): 356.43
 Lawson Number (LN): 28744, 28020, 3706
 Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 7162551
 Tautomer ID (TAUTID): 7958547
 Entry Date (DED): 2000/05/16
 Update Date (DUPD): 2000/05/16



Field Availability:

| Code | Name | Occurrence |
|--------|----------------------------|------------|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 3 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |
| IR | Infrared Spectrum | 1 |
| MP | Melting Point | 1 |
| NMR | Nuclear Magnetic Resonance | 2 |
| PHARM | Pharmacological Data | 1 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|-------|-------------------------------|------------|
| RX | Reaction Documents | 1 |
| RXPRO | Substance is Reaction Product | 1 |

=> d rx 139 28

L39 ANSWER 28 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:

RX

Reaction ID (.ID): 8532860
 Reactant BRN (.RBRN): 7432249, 4291410
 Reactant (.RCT): 8-phenyl-1,2,3,6-tetrahydro-6,7-diaza-cyclopentanaphthalen-5-one, 1-(2-chloro-ethyl)-1H-imidazole
 Product BRN (.PBRN): 8441980
 Product (.PRO): 6-(2-imidazol-1-yl-ethyl)-8-phenyl-1,2,3,6-tetrahydro-6,7-diaza-cyclopentanaphthalen-5-one
 No. of React. Details (.NVAR): 1

Reaction Details:

RX

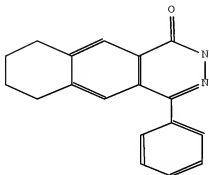
Reaction RID (.RID): 8532860.1
 Reaction Classification (.CL): Multistage
 Yield (.YDT): 68 percent (BRN=8441980)
 Nr. of Stages (.SNR): 2
 Stage 1
 Reagent (.RGT): NaH
 Solvent (.SOL): dimethylformamide
 Time (.TIM): 1 hour(s)
 Temperature (.T): 20 Cel
 Reaction Type (.TYP): deprotonation
 Stage 2
 Stage reactant (.SRCT): 1-(2-chloro-ethyl)-1#H!-imidazole
 Stage Reactant BRN (.SRBRN): 4291410
 Solvent (.SOL): dimethylformamide
 Time (.TIM): 14 hour(s)
 Temperature (.T): 70 Cel
 Reaction Type (.TYP): Substitution
 Reference(s):
 1. Haider, Norbert; Hartmann, Rolf W.; Steinwender, Andreas, Arch.Pharm.(Weinheim Ger.), CODEN: ARPMAS, 332(11), <1999>, 408 - 409; BABS-6205172

=> d ide 139 29

L39 ANSWER 29 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN): 7434131
 Chemical Name (CN): 6,7,8,9-tetrahydro-4-phenylbenzo<g>phthalazin-1(2H)-one
 Autonom Name (AUN): 4-phenyl-6,7,8,9-tetrahydro-2H-benzo<g>phtalazin-1-one
 Molec. Formula (MF): C18 H16 N2 O
 Molecular Weight (MW): 276.34
 Lawson Number (LN): 28745
 Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 6358917
 Tautomer ID (TAUTID): 72792
 Beilstein Citation (BSO): 6-24

10/772,445

Entry Date (DED):
Update Date (DUPD):1996/08/09
2000/05/16

Field Availability:

| Code | Name | Occurrence |
|--------|----------------------------|------------|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 1 |
| FS | File Segment | 1 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| BSO | Beilstein Citation | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |
| IR | Infrared Spectrum | 1 |
| MP | Melting Point | 1 |
| NMR | Nuclear Magnetic Resonance | 1 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|-------|--------------------------------|------------|
| RX | Reaction Documents | 3 |
| RXREA | Substance is Reaction Reactant | 2 |
| RXPRO | Substance is Reaction Product | 1 |

=> d rx 139 29

L39 ANSWER 29 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:
RX

10/772,445

Reaction ID (.ID): 4417477
 Reactant BRN (.RBRN): 1215280, 114797
 Reactant (.RCT): 4-phenyl-2H-pyridazino<4,5-d>pyridazin-1-one, 1-cyclohex-1-enyl-pyrrolidine
 Product BRN (.PBRN): 7434131
 Product (.PRO): 6,7,8,9-tetrahydro-4-phenylbenzo<g>phthalazin-1(2H)-one
 No. of React. Details (.NVAR): 1

Reaction Details:

RX
 Reaction RID (.RID): 4417477.1
 Reaction Classification (.CL): Preparation
 Reagent (.RGT): 2.) AcOH
 Other Conditions (.COND): 1.) 1,4-dioxane, reflux, 1 h, 2.) 1-propanol, reflux, 24 h
 Note(s) (.COM): Yield given. Multistep reaction
 Reference(s):
 1. Haider, Norbert, Heterocycles, CODEN: HTCYAM, 41(11), <1995>, 2519-2526; BABS-6008956

Reaction:

RX
 Reaction ID (.ID): 8533023
 Reactant BRN (.RBRN): 7434131, 4291410
 Reactant (.RCT): 6,7,8,9-tetrahydro-4-phenylbenzo<g>phthalazin-1(2H)-one, 1-(2-chloro-ethyl)-1H-imidazole
 Product BRN (.PBRN): 8444536
 Product (.PRO): 2-(2-imidazol-1-yl-ethyl)-4-phenyl-6,7,8,9-tetrahydro-2H-benzo<g>phthalazin-1-one
 No. of React. Details (.NVAR): 1

Reaction Details:

RX
 Reaction RID (.RID): 8533023.1
 Reaction Classification (.CL): Multistage
 Yield (.YDT): 70 percent (BRN=8444536)
 Nr. of Stages (.SNR): 2
 Stage 1
 Reagent (.RGT): NaH
 Solvent (.SOL): dimethylformamide
 Time (.TIM): 1 hour(s)
 Temperature (.T): 20 Cel
 Reaction Type (.TYP): deprotonation
 Stage 2
 Stage reactant (.SRCT): 1-(2-chloro-ethyl)-1H-imidazole
 Stage Reactant BRN (.SRBRN): 4291410
 Solvent (.SOL): dimethylformamide
 Time (.TIM): 14 hour(s)
 Temperature (.T): 70 Cel
 Reaction Type (.TYP): Substitution
 Reference(s):
 1. Haider, Norbert; Hartmann, Rolf W.; Steinwender, Andreas, Arch.Pharm.(Weinheim Ger.), CODEN: ARPMAS, 332(11), <1999>, 408 - 409; BABS-6205172

Reaction:

RX
 Reaction ID (.ID): 4637798

10/772,445

Reactant BRN (.RBRN): 7434131
 Reactant (.RCT): 6,7,8,9-tetrahydro-4-phenylbenzo<g>phthalazin-1(2H)-one
 Product BRN (.PBRN): 7647989
 Product (.PRO): 1-chloro-6,7,8,9-tetrahydro-4-phenylbenzo<g>phthalazine
 No. of React. Details (.NVAR): 1

Reaction Details:

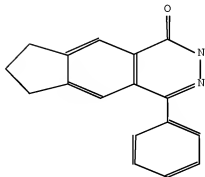
RX

Reaction RID (.RID): 4637798.1
 Reaction Classification (.CL): Preparation
 Yield (.YDT): 50 percent (BRN=7647989)
 Reagent (.RGT): POC13, N,N-diethylaniline
 Time (.TIM): 2 hour(s)
 Temperature (.T): 90 Cel
 Reference(s):
 1. Haider, Norbert; Steinwender, Andreas, Sci.Pharm., CODEN: SCPHA4, 64(3/4), <1996>, 399-406; BABS-6049366

=> d ide 139 30

L39 ANSWER 30 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN): 7432249
 Chemical Name (CN): 2,6,7,8-tetrahydro-4-phenyl-1H-cyclopenta<g>phthalazin-1-one
 Autonom Name (AUN): 8-phenyl-1,2,3,6-tetrahydro-6,7-diaza-cyclopentanaphthalen-5-one
 Molec. Formula (MF): C17 H14 N2 O
 Molecular Weight (MW): 262.31
 Lawson Number (LN): 28744
 Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 6355731
 Tautomer ID (TAUTID): 7055539
 Beilstein Citation (BSO): 6-24
 Entry Date (DED): 1996/08/09
 Update Date (DUPD): 2000/05/16



Field Availability:

| Code | Name | Occurrence |
|--------|----------------------------|------------|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| AUN | Autononname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 1 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| BSO | Beilstein Citation | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |
| IR | Infrared Spectrum | 1 |
| MP | Melting Point | 1 |
| NMR | Nuclear Magnetic Resonance | 2 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|-------|--------------------------------|------------|
| RX | Reaction Documents | 3 |
| RXREA | Substance is Reaction Reactant | 2 |
| RXPRO | Substance is Reaction Product | 1 |

=> d rx 139 30

L39 ANSWER 30 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:

RX
 Reaction ID (.ID): 4416653
 Reactant BRN (.RBRN): 1215280, 109824
 Reactant (.RCT): 4-phenyl-2H-pyridazino<4,5-d>pyridazin-1-one, 1-cyclopent-1-enyl-pyrrolidine
 Product BRN (.PBRN): 7432249
 Product (.PRO): 8-phenyl-1,2,3,6-tetrahydro-6,7-diaza-cyclopentanaphthalen-5-one
 No. of React. Details (.NVAR): 1

Reaction Details:

RX
 Reaction RID (.RID): 4416653.1
 Reaction Classification (.CL): Preparation
 Reagent (.RGT): 2.) AcOH
 Other Conditions (.COND): 1.) 1,4-dioxane, reflux, 1 h, 2.) 1-propanol, reflux, 24 h
 Note(s) (.COM): Yield given. Multistep reaction
 Reference(s):
 1. Haider, Norbert, Heterocycles, CODEN: HTCYAM, 41(11), <1995>, 2519-2526; BABS-6008956

Reaction:

RX

| | |
|--------------------------------|--|
| Reaction ID (.ID): | 8532860 |
| Reactant BRN (.RBRN): | 7432249, 4291410 |
| Reactant (.RCT): | 8-phenyl-1,2,3,6-tetrahydro-6,7-diaza-cyclopentanaphthalen-5-one, 1-(2-chloro-ethyl)-1H-imidazole |
| Product BRN (.PBRN): | 8441980 |
| Product (.PRO): | 6-(2-imidazol-1-yl-ethyl)-8-phenyl-1,2,3,6-tetrahydro-6,7-diaza-cyclopentanaphthalen-5-one |
| No. of React. Details (.NVAR): | 1 |

Reaction Details:

RX

| | |
|--|-----------------------------------|
| Reaction RID (.RID): | 8532860.1 |
| Reaction Classification (.CL): | Multistage |
| Yield (.YDT): | 68 percent (BRN=8441980) |
| Nr. of Stages (.SNR): | 2 |
| Stage 1 | |
| Reagent (.RGT): | NaH |
| Solvent (.SOL): | dimethylformamide |
| Time (.TIM): | 1 hour(s) |
| Temperature (.T): | 20 Cel |
| Reaction Type (.TYP): | deprotonation |
| Stage 2 | |
| Stage reactant (.SRCT): | 1-(2-chloro-ethyl)-1#H!-imidazole |
| Stage Reactant BRN (.SRBRN): | 4291410 |
| Solvent (.SOL): | dimethylformamide |
| Time (.TIM): | 14 hour(s) |
| Temperature (.T): | 70 Cel |
| Reaction Type (.TYP): | Substitution |
| Reference(s): | |
| 1. Haider, Norbert; Hartmann, Rolf W.; Steinwender, Andreas, Arch.Pharm.(Weinheim Ger.), CODEN: ARPMAS, 332(11), <1999>, 408 - 409; BABS-6205172 | |

Reaction:

RX

| | |
|--------------------------------|---|
| Reaction ID (.ID): | 4637784 |
| Reactant BRN (.RBRN): | 7432249 |
| Reactant (.RCT): | 8-phenyl-1,2,3,6-tetrahydro-6,7-diaza-cyclopentanaphthalen-5-one |
| Product BRN (.PBRN): | 7645601 |
| Product (.PRO): | 5-chloro-8-phenyl-2,3-dihydro-1H-6,7-diaza-cyclopentanaphthalene |
| No. of React. Details (.NVAR): | 1 |

Reaction Details:

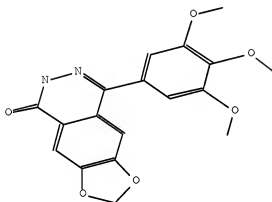
RX

| | |
|---|--|
| Reaction RID (.RID): | 4637784.1 |
| Reaction Classification (.CL): | Preparation |
| Yield (.YDT): | 36 percent (BRN=7645601) |
| Reagent (.RGT): | POCl ₃ , N,N-diethylaniline |
| Time (.TIM): | 2 hour(s) |
| Temperature (.T): | 90 Cel |
| Reference(s): | |
| 1. Haider, Norbert; Steinwender, Andreas, Sci.Pharm., CODEN: SCPHA4, 64(3/4), <1996>, 399-406; BABS-6049366 | |

=> d ide 139 31

L39 ANSWER 31 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN): 347858
 Chemical Name (CN): 8-(3,4,5-trimethoxy-phenyl)-6H-<1,3>dioxol
 o<4,5-g>phthalazin-5-one
 Autonom Name (AUN): 8-(3,4,5-trimethoxy-phenyl)-6H-<1,3>dioxol
 o<4,5-g>phthalazin-5-one
 Molec. Formula (MF): C18 H16 N2 O6
 Molecular Weight (MW): 356.33
 Lawson Number (LN): 32377, 289
 Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 337329
 Tautomer ID (TAUTID): 359024
 Beilstein Citation (BSO): 4-27-00-08904
 Entry Date (DED): 1988/06/27
 Update Date (DUPD): 1992/05/13



Field Availability:

| Code | Name | Occurrence |
|--------|--------------------|------------|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 2 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| BSO | Beilstein Citation | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |

MP Melting Point

1

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|-------|--------------------------------|------------|
| RX | Reaction Documents | 3 |
| RXREA | Substance is Reaction Reactant | 2 |
| RXPRO | Substance is Reaction Product | 1 |

=> d rx 139 31

L39 ANSWER 31 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:

RX

| | |
|--------------------------------|--|
| Reaction ID (.ID): | 5569349 |
| Reactant (.RCT): | 6-<3.4.5-trimethoxy-benzoyl>-benzo<1.3>dioxole-5-carboxylic acid |
| Product BRN (.PBRN): | 347858 |
| Product (.PRO): | 8-(3,4,5-trimethoxy-phenyl)-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one |
| No. of React. Details (.NVAR): | 1 |

Reaction Details:

RX

| | |
|---|-----------------------------|
| Reaction RID (.RID): | 5569349.1 |
| Reaction Classification (.CL): | Preparation (half reaction) |
| Reagent (.RGT): | ethanol, N2H4+H2O |
| Note(s) (.COM): | Handbook |
| Reference(s): | |
| 1. Noguchi; Kawanami, Yakugaku Zasshi, CODEN: YKKZAJ, 60, <1940>, 629, 634, Chem.Abstr., <1953>, 6386 | |

Reaction:

RX

| | |
|--------------------------------|--|
| Reaction ID (.ID): | 5741896 |
| Reactant BRN (.RBRN): | 347858 |
| Reactant (.RCT): | 8-(3,4,5-trimethoxy-phenyl)-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one |
| Product (.PRO): | oxime C18H17N3O6 |
| No. of React. Details (.NVAR): | 1 |

Reaction Details:

RX

| | |
|---|------------------------------------|
| Reaction RID (.RID): | 5741896.1 |
| Reaction Classification (.CL): | Chemical behaviour (half reaction) |
| Note(s) (.COM): | Handbook |
| Reference(s): | |
| 1. Noguchi; Kawanami, Yakugaku Zasshi, CODEN: YKKZAJ, 60, <1940>, 629, 634, Chem.Abstr., <1953>, 6386 | |

Reaction:

RX

| | |
|-----------------------|--|
| Reaction ID (.ID): | 521344 |
| Reactant BRN (.RBRN): | 347858 |
| Reactant (.RCT): | 8-(3,4,5-trimethoxy-phenyl)-6H-<1,3>dioxolo<4,5-g>phthalazin-5-one |

10/772,445

Product BRN (.PBRN): 355497
 Product (.PRO): 8-(3,4,5-trimethoxy-phenyl)-6H-<1,3>dioxol
 o<4,5-g>phthalazin-5-one oxime
 No. of React. Details (.NVAR): 1

Reaction Details:

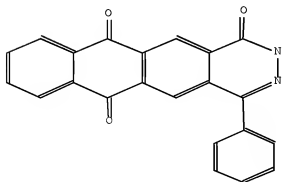
RX

Reaction RID (.RID): 521344.1
 Reaction Classification (.CL): Preparation
 Note(s) (.COM): Handbook
 Reference(s):
 1. Noguchi; Kawanami, Yakugaku Zasshi, CODEN: YKKZAJ, 60, <1940>, 629,
 634, Chem.Abstr., <1953>, 6386

=> d ide 139 32

L39 ANSWER 32 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN): 43230
 Chemical Name (CN): 4-phenyl-2H-naphtho<2,3-g>phthalazine-1,6,
 11-trione
 Autonom Name (AUN): 4-phenyl-2H-2,3-diaza-naphthacene-1,6,11-t
 rione
 Molec. Formula (MF): C22 H12 N2 O3
 Molecular Weight (MW): 352.35
 Lawson Number (LN): 28973
 Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 61454
 Tautomer ID (TAUTID): 82402
 Beilstein Citation (BSO): 4-24-00-02134
 Entry Date (DED): 1988/06/27
 Update Date (DUPD): 1992/05/13



Field Availability:

Code Name

Occurrence

| | | |
|--------|------------------------------|---|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 1 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| BSO | Beilstein Citation | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |
| CPD | Crystal Property Description | 1 |
| MP | Melting Point | 1 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|-------|-------------------------------|------------|
| RX | Reaction Documents | 1 |
| RXPRO | Substance is Reaction Product | 1 |

=> d rx 139 32

L39 ANSWER 32 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:

RX
 Reaction ID (.ID): 514252
 Reactant BRN (.RBRN): 3443618
 Reactant (.RCT): 3-benzoyl-9,10-dioxo-9,10-dihydro-anthracene-2-carboxylic acid
 Product BRN (.PBRN): 43230
 Product (.PRO): 4-phenyl-2H-naphtho<2,3-g>phthalazine-1,6,11-trione
 No. of React. Details (.NVAR): 1

Reaction Details:

RX
 Reaction RID (.RID): 514252.1
 Reaction Classification (.CL): Preparation
 Reagent (.RGT): ethanol, N2H4+H2O
 Temperature (.T): 120 Cel
 Note(s) (.COM): Handbook
 Reference(s):
 1. Seka et al., Monatsh.Chem., CODEN: MOCMB7, 57, <1931>, 86,93

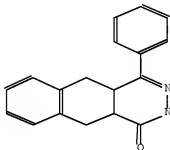
=> d ide 139 33

L39 ANSWER 33 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN): 28738
 Beilstein Pref. RN (BPR): 109892-05-9
 CAS Reg. No. (RN): 109892-05-9
 Chemical Name (CN): 4-phenyl-4a,5,10,10a-tetrahydro-2H-benzo<g

10/772,445

Autonom Name (AUN): >phthalazin-1-one
 4-phenyl-4a,5,10,10a-tetrahydro-2H-benzo<g
 >phthalazin-1-one
 Molec. Formula (MF): C18 H16 N2 O
 Molecular Weight (MW): 276.34
 Lawson Number (LN): 28745
 Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 34762
 Tautomer ID (TAUTID): 72792
 Beilstein Citation (BSO): 4-24-00-00740
 Entry Date (DED): 1988/06/27
 Update Date (DUPD): 1992/05/13



Field Availability:

| Code | Name | Occurrence |
|--------|------------------------|------------|
| BRN | Beilstein Records | 1 |
| BPR | Beilstein Preferred RN | 1 |
| RN | CAS Registry Number | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 1 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| BSO | Beilstein Citation | 1 |
| DED | Entry Date | 1 |
| DUPD | Update Date | 1 |
| MP | Melting Point | 1 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|-------|-------------------------------|------------|
| RX | Reaction Documents | 1 |
| RXPRO | Substance is Reaction Product | 1 |

=> d rx 139 33

L39 ANSWER 33 OF 33 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Reaction:

RX

| | |
|--------------------------------|---|
| Reaction ID (.ID): | 5533353 |
| Reactant (.RCT): | 3-benzoyl-1,2,3,4-tetrahydro-naphthalene-2-carboxylic acid |
| Product BRN (.PBRN): | 28738 |
| Product (.PRO): | 4-phenyl-4a,5,10,10a-tetrahydro-2H-benzo<g>phthalazin-1-one |
| No. of React. Details (.NVAR): | 1 |

Reaction Details:

RX

| | |
|--------------------------------|--|
| Reaction RID (.RID): | 5533353.1 |
| Reaction Classification (.CL): | Preparation (half reaction) |
| Reagent (.RGT): | N2H4+H2O |
| Note(s) (.COM): | Handbook |
| Reference(s): | 1. Buchta; Egger, Chem.Ber., CODEN: CHBEAM, 90, <1957>, 2760, 2763 |

```
=> d que nos 130
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L8      STR
L10     56 SEA FILE=REGISTRY SSS FUL L8
L13     STR
L15     37 SEA FILE=REGISTRY SUB=L10 SSS FUL L13
L19     QUE SPE=ON  ABB=ON  PLU=ON  UPASANI, R?/AU
L20     QUE SPE=ON  ABB=ON  PLU=ON  CAI, S?/AU
L21     QUE SPE=ON  ABB=ON  PLU=ON  LAN, N?/AU
L22     QUE SPE=ON  ABB=ON  PLU=ON  WANG, Y?/AU
L23     QUE SPE=ON  ABB=ON  PLU=ON  FIELD, G?/AU
L24     QUE SPE=ON  ABB=ON  PLU=ON  FICK, D?/AU
L25     QUE SPE=ON  ABB=ON  PLU=ON  (COCENSYS OR (PURDUE(1W)PHAR
MA) OR (EURO(1W)CELTIQUE))/CS,SO,PA
L27     17 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L15
L28     1 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L27 AND (L19 OR L20
OR L21 OR L22 OR L23 OR L24 OR L25)
L29     1 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L1 AND L28
L30     1 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  (L28 OR L29)
```

```
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L33     3 S L32 AND L19-L25
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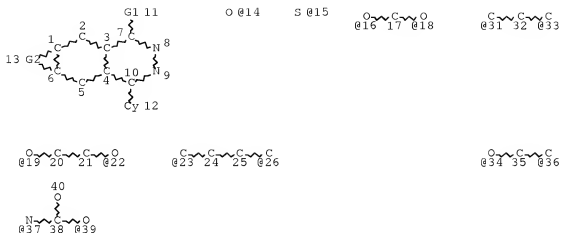
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=> d que nos 133
L8      STR
L10     56 SEA FILE=REGISTRY SSS FUL L8
L13     STR
L15     37 SEA FILE=REGISTRY SUB=L10 SSS FUL L13
L19     QUE SPE=ON  ABB=ON  PLU=ON  UPASANI, R?/AU
L20     QUE SPE=ON  ABB=ON  PLU=ON  CAI, S?/AU
L21     QUE SPE=ON  ABB=ON  PLU=ON  LAN, N?/AU
L22     QUE SPE=ON  ABB=ON  PLU=ON  WANG, Y?/AU
L23     QUE SPE=ON  ABB=ON  PLU=ON  FIELD, G?/AU
L24     QUE SPE=ON  ABB=ON  PLU=ON  FICK, D?/AU
L25     QUE SPE=ON  ABB=ON  PLU=ON  (COCENSYS OR (PURDUE(1W)PHAR
MA) OR (EURO(1W)CELTIQUE))/CS,SO,PA
L32     9 SEA L15
L33     3 SEA L32 AND (L19 OR L20 OR L21 OR L22 OR L23 OR L24 OR L25)
```

```
=> d que nos 142
L13     STR
L19     QUE SPE=ON  ABB=ON  PLU=ON  UPASANI, R?/AU
L20     QUE SPE=ON  ABB=ON  PLU=ON  CAI, S?/AU
L21     QUE SPE=ON  ABB=ON  PLU=ON  LAN, N?/AU
L22     QUE SPE=ON  ABB=ON  PLU=ON  WANG, Y?/AU
L23     QUE SPE=ON  ABB=ON  PLU=ON  FIELD, G?/AU
L24     QUE SPE=ON  ABB=ON  PLU=ON  FICK, D?/AU
L25     QUE SPE=ON  ABB=ON  PLU=ON  (COCENSYS OR (PURDUE(1W)PHAR
MA) OR (EURO(1W)CELTIQUE))/CS,SO,PA
L41     4 SEA FILE=CHEMINFORMRX SSS FUL L13 (      8 REACTIONS)
L42     0 SEA FILE=CHEMINFORMRX SPE=ON  ABB=ON  PLU=ON  L41 AND (L19 OR
L20 OR L21 OR L22 OR L23 OR L24 OR L25)
```


=> d que 145

L13

STR



VAR G1=14/15

VAR G2=16-6 18-1/19-6 22-1/31-6 33-1/23-6 26-1/34-6 36-1/36-6 34-1/37-6 3

9-1/39-6 37-1

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 14

CONNECT IS E1 RC AT 15

CONNECT IS E1 RC AT 40

DEFAULT MLEVEL IS ATOM

GGCAT IS UNS AT 12

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 36

STEREO ATTRIBUTES: NONE

L45 8 SEA FILE=WPIX SSS FUL L13

=> d que nos 150

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L2      1 SEA FILE=WPIX SPE=ON  ABB=ON  PLU=ON  US2004-772445/APPS
L13     STR
L19     QUE  SPE=ON  ABB=ON  PLU=ON  UPASANI, R?/AU
L20     QUE  SPE=ON  ABB=ON  PLU=ON  CAI, S?/AU
L21     QUE  SPE=ON  ABB=ON  PLU=ON  LAN, N?/AU
L22     QUE  SPE=ON  ABB=ON  PLU=ON  WANG, Y?/AU
L23     QUE  SPE=ON  ABB=ON  PLU=ON  FIELD, G?/AU
L24     QUE  SPE=ON  ABB=ON  PLU=ON  FICK, D?/AU
L25     QUE  SPE=ON  ABB=ON  PLU=ON  (COCENSYS OR (PURDUE(1W)PHAR
      MA) OR (EURO(1W)CELTIQUE))/CS,SO,PA
L45     8 SEA FILE=WPIX SSS FUL L13
L46     1 SEA FILE=WPIX SPE=ON  ABB=ON  PLU=ON  (RA00N1/DCN OR RA00N2/DCN
      OR RA00N3/DCN OR RA00N4/DCN OR RA00N5/DCN OR RA00N6/DCN OR
      RA00N7/DCN OR RA00N8/DCN) OR L45/DCR
L47     1 SEA FILE=WPIX SPE=ON  ABB=ON  PLU=ON  L46 AND (L19 OR L20 OR
      L21 OR L22 OR L23 OR L24 OR L25)
L49     1 SEA FILE=WPIX SPE=ON  ABB=ON  PLU=ON  L47 AND L2

```

L50 1 SEA FILE=WPIX SPE=ON ABB=ON PLU=ON L47 OR L49

=> d his l54

(FILE 'HCAPLUS', WPIX, MEDLINE, BIOSIS, EMBASE, PASCAL, CABA, CEABA-VTB, LIFESCI, BIOENG, BIOTECHNO, BIOTECHDS, DRUGU, DRUGB, VETU, VETB, SCISEARCH, CONFSCI, DISSABS, RDISCLOSURE' ENTERED AT 15:39:34 ON 04 DEC 2008)

L54 15 S L52 AND L25

=> d que l54

L19 QUE SPE=ON ABB=ON PLU=ON UPASANI, R?/AU
 L20 QUE SPE=ON ABB=ON PLU=ON CAI, S?/AU
 L21 QUE SPE=ON ABB=ON PLU=ON LAN, N?/AU
 L22 QUE SPE=ON ABB=ON PLU=ON WANG, Y?/AU
 L23 QUE SPE=ON ABB=ON PLU=ON FIELD, G?/AU
 L24 QUE SPE=ON ABB=ON PLU=ON FICK, D?/AU
 L25 QUE SPE=ON ABB=ON PLU=ON (COCENSYS OR (PURDUE(1W)PHAR
 MA) OR (EURO(1W)CELTIQUE))/CS,SO,PA
 L52 164 SEA (L19 OR L20 OR L21 OR L22 OR L23 OR L24 OR L25) AND
 ?QUINAZOLIN?/IT,TI,CC,CT,ST,STP
 L54 15 SEA L52 AND L25

=> dup rem l30 l33 l42 l50 l54

L42 HAS NO ANSWERS

DUPLICATE IS NOT AVAILABLE IN 'CHEMINFORMRX, RDISCLOSURE'.

ANSWERS FROM THESE FILES WILL BE CONSIDERED UNIQUE

FILE 'HCAPLUS' ENTERED AT 15:58:57 ON 04 DEC 2008

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PROCESSING COMPLETED FOR L30

PROCESSING COMPLETED FOR L33

PROCESSING COMPLETED FOR L42

PROCESSING COMPLETED FOR L50

PROCESSING COMPLETED FOR L54

L56 12 DUP REM L30 L33 L42 L50 L54 (8 DUPLICATES REMOVED)

ANSWERS '1-6' FROM FILE HCAPLUS

ANSWERS '7-9' FROM FILE USPATFULL

ANSWERS '10-11' FROM FILE BIOSIS

10/772,445

ANSWER '12' FROM FILE SCISEARCH

=> file stnguide

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FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Nov 21, 2008 (20081121/UP).

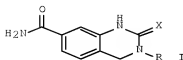
=> d ibib ed abs hitind hitstr l-6
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 CONTINUE? (Y)/N:y

L56 ANSWER 1 OF 12 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 2
 ACCESSION NUMBER: 2004:657939 HCAPLUS Full-text
 TITLE: Quinazolinones and benzothiazinones as novel
 sodium channel blockers
 AUTHOR(S): Victory, Sam F.; Sun, Qun; Limberis, Jim; Kyle, Donald
 J.
 CORPORATE SOURCE: Discovery Research, Purdue Pharma,
 L.P., Cranbury, NJ, 08512, USA
 SOURCE: Abstracts of Papers, 228th ACS National Meeting,
 Philadelphia, PA, United States, August 22-26, 2004
 (2004), MEDI-075. American Chemical Society:
 Washington, D. C.
 CODEN: 69FTZ8
 DOCUMENT TYPE: Conference; Meeting Abstract
 LANGUAGE: English
 ED Entered STN: 15 Aug 2004

AB V102862 is a potent state-dependent sodium channel blocker ($K_i = 370$ nM, rBIIa) that has been shown to be efficacious in the Chung model of neuropathic pain. Toward the discovery of a second-generation compound having an improved pharmaceutical profile, we embarked on a systematic structure-activity investigation aimed at replacing the semicarbazone moiety of V102862 with various heterocycles as a bioisosteric replacement. Our labs. have reported on several series of high affinity sodium channel blockers as part of this effort, including a series of compds. containing a thiazolidinone ring system as a replacement. Some of the most potent compds. in the thiazolidinone series possessed a hydrophobic aryl ether moiety, similar to V102862, and also a piperidinylethylamine moiety. To further explore the bioisosteric replacement of the semicarbazone moiety of V102862, several addnl. series of compds. were synthesized including those having a quinazolin-4(3H)-one or a 2,3-dihydro-benzothiazin-4-one core ring system. Within each of these new series, the optimized piperidinylethylamine group of the thiazolidinone series was held constant while the hydrophobic aryl ether moiety was varied, generating potent sodium channel blockers in each series. Details of the synthesis and SAR of analogs will be presented.

L56 ANSWER 2 OF 12 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 4
 ACCESSION NUMBER: 2001:420169 HCAPLUS Full-text
 DOCUMENT NUMBER: 135:226951
 TITLE: Solid-phase synthesis of 3,4-dihydro-2(1H)-
quinazolinones and 3,4-dihydro-1H-
quinazolin-2-thiones
 AUTHOR(S): Sun, Q.; Zhou, X.; Kyle, D. J.
 CORPORATE SOURCE: Department of Computational, Combinatorial and
 Medicinal Chemistry, Purdue Pharma
 LP, Cranbury, NJ, 08512, USA
 SOURCE: Tetrahedron Letters (2001), 42(25), 4119-4121
 CODEN: TELEAY; ISSN: 0040-4039
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 135:226951

ED Entered STN: 11 Jun 2001
GI

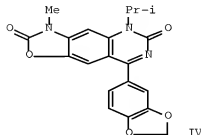
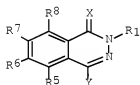
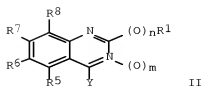
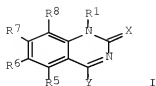


- AB Dihydroquinazolinones and dihydroquinazolinethiones I [R = PhCH₂, 3-pyridylmethyl, PhCH(Me), 4-MeOC₆H₄CH₂, 4-MeOC₆H₄CH₂CH₂, 1-naphthylmethyl, Ph₂CHCH₂, 1-benzyl-4-piperidinemethyl, 2-(4-morpholinyl)ethyl, Me₂NCH₂CH₂, Me₂CHCH₂; X = O, S] are prepared on solid phase. E.g., Fmoc-Rink resin was deprotected with piperidine and treated with 4-(bromomethyl)-3-nitrobenzoic acid with 1-hydroxybenzotriazole and diisopropyl carbodiimide to give the resin-bound benzamide; addition of benzylamine gave a resin-bound (benzylaminomethyl)nitrobenzamide which was reduced with tin (II) chloride to give a resin-bound (benzylaminomethyl)aminobenzamide. E.g., treatment of the resin-bound (benzylaminomethyl)aminobenzamide with disuccinimidyl carbonate in DMF followed by cleavage of the resin with trifluoroacetic acid gave the dihydroquinazolinones I (X = O) in 73-100% yields and 60-95% purities, while treatment of the resin-bound (benzylaminomethyl)aminobenzamide with thiocarbonyldiimidazole followed by cleavage of the resin with trifluoroacetic acid gave the dihydroquinazolinethiones I (X = S) in 72-97% yields and 60-89% purities.
- CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
- ST hydroquinazolinones hydroquinazolinethione solid phase prepn; quinazolinone quinazolinethione solid phase prepn
- IT Solid phase synthesis
(solid-phase preparation of substituted quinazolinones and quinazolinethiones)
- IT Amines, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(solid-phase preparation of substituted quinazolinones and quinazolinethiones)
- IT 55-81-2, 4-Methoxyphenethyl amine 78-81-9, Isobutylamine 100-46-9, Benzylamine, reactions 108-00-9, 2-(Dimethylamino)ethylamine 118-31-0, 1-Naphthylmethylamine 618-36-0, α -Methylbenzylamine 2038-03-1, 2-(4-Morpholinyl)ethylamine 2393-23-9, 4-Methoxybenzylamine 3731-52-0, 3-Pyridylmethylamine 5586-73-2, 3,3-Diphenylpropylamine 50541-93-0 55715-03-2D, 3-Nitro-4-(bromomethyl)benzoic acid, resin-bound 84418-43-9D, resin-bound
- RL: RCT (Reactant); RACT (Reactant or reagent)
(solid-phase preparation of substituted quinazolinones and quinazolinethiones)
- IT 358718-76-0P 358718-77-1P 358718-78-2P 358718-79-3P 358718-80-6P
358718-81-7P 358718-82-8P 358718-83-9P 358718-84-0P 358718-85-1P
358718-86-2P 358718-87-3P 358718-88-4P 358718-89-5P 358718-90-8P
358718-91-9P 358718-92-0P 358718-93-1P 358718-94-2P 358718-95-3P
358718-96-4P 358718-97-5P
- RL: SPN (Synthetic preparation); PREP (Preparation)
(solid-phase preparation of substituted quinazolinones and quinazolinethiones)
- REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L56 ANSWER 3 OF 12 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 5
 ACCESSION NUMBER: 1999:576785 HCAPLUS Full-text
 DOCUMENT NUMBER: 131:214294
 TITLE: Preparation of substituted quinazolines and heterocyclic analogs as antagonists or positive modulators of AMPA receptors
 INVENTOR(S): Upasani, Ravi; Cai, Sui X.; Lan, Nancy C.; Wang, Yan; Field, George; Pick, David B.
 PATENT ASSIGNEE(S): Cocossys, Inc., USA
 SOURCE: PCT Int. Appl., 117 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|--------------|
| WO 9944612 | A1 | 19990910 | WO 1999-US4609 | 19990302 |
| W: JP, US | | | | |
| RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| EP 1066039 | A1 | 20010110 | EP 1999-911063 | 19990302 |
| R: BE, CH, DE, ES, FR, GB, IT, LI, NL, IE | | | | |
| JP 2002505288 | T | 20020219 | JP 2000-534214 | 19990302 |
| US 6465472 | B1 | 20021015 | US 2000-654839 | 20000901 |
| US 20030033089 | A1 | 20030213 | US 2002-219755 | 20020816 |
| US 6765006 | B2 | 20040720 | | |
| US 20040162299 | A1 | 20040819 | US 2004-772445 | 20040206 <-- |
| PRIORITY APPLN. INFO.: | | | | |
| US 1998-76451P P 19980302 | | | | |
| WO 1999-US4609 W 19990302 | | | | |
| US 2000-654839 A3 20000901 | | | | |
| US 2002-219755 A3 20020816 | | | | |
| OTHER SOURCE(S): MARPAT 131:214294 | | | | |
| ED Entered STN: 14 Sep 1999 | | | | |
| GI | | | | |



AB Substituted quinazolines and heterocyclic analogs (I, II, and III) [R1 = (un)substituted alkyl, alkenyl, or alkynyl; R5 and R8 = independently H, halogen, NO2, NH2, CN, alkanoylamido, OH, SH, alkoxy, (un)substituted alkyl, (hetero)aryl, heterocyclic, alkenyl, or alkynyl, etc.; R6 and R7 taken together = 5- or 6-membered carbocyclic or heterocyclic ring; X = O or S; Y = (hetero)aryl; n and m = independently 0 or 1] were prepared as antagonists or pos. modulators of AMPA receptors for treatment, prevention, or amelioration of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia. Thus, 3-methyl-5-nitro-2(3H)-benzoxazolone was reduced to the amine over Pt/C in glacial acetic acid. Na cyanoborohydride was added to a suspension of the amine, THF, acetic acid, and acetone followed by treatment with NaOH and water to precipitate 5-(isopropylamino)-3-methyl-2(3H)-benzoxazolone. The substituted amine was converted to the ureido derivative by stirring with KCN in glacial acetic acid for 5 days. The urea was cyclized with piperonal in benzene and methanesulfonic acid to form the 3,4-dihydrooxazolo[4,5-g]quinazolin-2(1H)-one. The product was reduced by addition of KMnO4 in H2O followed by treatment with formalin to yield 1-isopropyl-4-(3,4-methylenedioxiphenyl)-8-methyl-7-oxoxazolo[4,5-g]quinazolin-2(1H)-one (IV). Selected compds. of the invention were tested for preferred binding to AMPA receptors and exhibited IC50 values ranging from 0.2 to 13 μ M. The anticonvulsant activity of the AMPA antagonists was evaluated in the Maximal Electroshock-induced Seizure (MES) test. MES ED50 values ranged from 1 to 10 mg/kg i.v.

IC ICM A61K031-50

ICS A61K031-505; C07D237-26; C07D239-70; C07D491-04; C07D491-048;
C07D491-056; C07D498-04

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1

| | | | | |
|-------------------------|--------------|--------------|--------------|--------------|
| IT 10368-14-6P | 33095-75-9P | 33095-79-3P | 33095-82-8P | 33095-94-2P |
| 34060-22-5P | 40484-04-6P | 59856-06-3P | 63546-19-0P | 85575-57-1P |
| 164526-15-2P | 243133-76-8P | 243133-77-9P | 243133-78-0P | 243133-79-1P |
| 243133-81-5P | 243133-82-6P | 243133-85-9P | 243133-86-0P | 243133-88-2P |
| 243133-90-6P | 243133-92-8P | 243133-94-0P | 243133-95-1P | 243133-96-2P |
| 243133-97-3P | 243133-98-4P | 243133-99-5P | 243134-07-8P | 243134-13-6P |
| 243134-40-9P | 243134-48-7P | 243134-49-8P | 243134-53-4P | 243134-58-9P |
| 243134-66-9P | 243134-73-8P | | | |

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU

(Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT
(Reactant or reagent); USES (Uses)

(target compound; preparation of substituted quinazolines and heterocyclic
analogs as antagonists or pos. modulators of AMPA receptors for
treatment of global ischemia, amyotrophic lateral sclerosis, acute or
chronic pain, or schizophrenia)

IT 13067-19-1P 33095-76-0P 33100-29-7P 40483-99-6P 119179-46-3P
243133-80-4P 243133-83-7P 243133-84-8P 243133-87-1P 243133-89-3P
243133-91-7P 243133-93-9P 243134-00-1P 243134-01-2P 243134-02-3P
243134-03-4P 243134-04-5P 243134-05-6P 243134-06-7P 243134-08-9P
243134-09-0P 243134-10-3P 243134-11-4P 243134-12-5P 243134-14-7P
243134-15-8P 243134-16-9P 243134-17-0P 243134-18-1P 243134-19-2P
243134-20-5P 243134-21-6P 243134-22-7P 243134-23-8P 243134-24-9P
243134-25-0P 243134-26-1P 243134-27-2P 243134-28-3P 243134-29-4P
243134-30-7P 243134-31-8P 243134-32-9P 243134-33-0P 243134-34-1P
243134-35-2P 243134-36-3P 243134-37-4P 243134-38-5P 243134-42-1P
243134-44-3P 243134-46-5P 243134-50-1P 243134-51-2P 243134-52-3P
243134-54-5P 243134-55-6P 243134-56-7P 243134-57-8P 243134-59-0P
243134-60-3P 243134-61-4P 243134-62-5P 243134-63-6P 243134-64-7P
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243134-87-4P 243134-88-5P 243134-89-6P 243134-90-9P 243134-91-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)

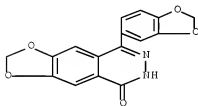
(target compound; preparation of substituted quinazolines and heterocyclic
analogs as antagonists or pos. modulators of AMPA receptors for
treatment of global ischemia, amyotrophic lateral sclerosis, acute or
chronic pain, or schizophrenia)

IT 243134-69-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT
(Reactant or reagent); USES (Uses)

(target compound; preparation of substituted quinazolines and heterocyclic
analogs as antagonists or pos. modulators of AMPA receptors for
treatment of global ischemia, amyotrophic lateral sclerosis, acute or
chronic pain, or schizophrenia)

RN 243134-66-9 HCAPLUS

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(1,3-benzodioxol-5-yl)- (CA
INDEX NAME)



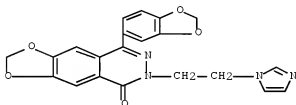
IT 243134-67-0P 243134-68-1P 243134-69-2P
243134-70-5P 243134-71-6P 243134-72-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(target compound; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)

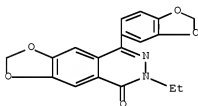
RN 243134-67-0 HCAPLUS

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(1,3-benzodioxol-5-yl)-6-[2-(1H-imidazol-1-yl)ethyl]- (CA INDEX NAME)



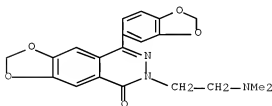
RN 243134-68-1 HCAPLUS

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(1,3-benzodioxol-5-yl)-6-ethyl- (CA INDEX NAME)



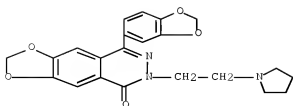
RN 243134-69-2 HCAPLUS

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(1,3-benzodioxol-5-yl)-6-[2-(dimethylamino)ethyl]- (CA INDEX NAME)

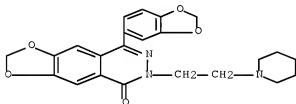


RN 243134-70-5 HCAPLUS

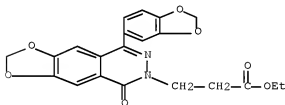
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(1,3-benzodioxol-5-yl)-6-[2-(1-pyrrolidinyl)ethyl]- (CA INDEX NAME)



RN 243134-71-6 HCAPLUS
 CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one,
 8-(1,3-benzodioxol-5-yl)-6-[2-(1-piperidinyl)ethyl]- (CA INDEX NAME)



RN 243134-72-7 HCAPLUS
 CN 1,3-Dioxolo[4,5-g]phthalazine-6(5H)-propanoic acid,
 8-(1,3-benzodioxol-5-yl)-5-oxo-, ethyl ester (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L56 ANSWER 4 OF 12 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2004:120836 HCAPLUS [Full-text](#)
 DOCUMENT NUMBER: 140:181460
 TITLE: Preparation of (piperidinylethyl)benzoheterocyclic
 compounds for use as sodium channel blockers
 INVENTOR(S): Sun, Qun; Kyle, Donald J.; Victory, Samuel F.
 PATENT ASSIGNEE(S): [Euro-Celtique](#) S.A., Luxembourg
 SOURCE: PCT Int. Appl., 58 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent

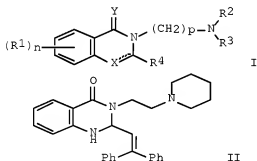
LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|------------|
| WO 2004013111 | A1 | 20040212 | WO 2003-US23791 | 20030730 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| US 20040152696 | A1 | 20040805 | US 2003-628487 | 20030729 |
| CA 2493737 | A1 | 20040212 | CA 2003-2493737 | 20030730 |
| AU 2003257015 | A1 | 20040223 | AU 2003-257015 | 20030730 |
| EP 1534690 | A1 | 20050601 | EP 2003-766980 | 20030730 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | | |
| BR 2003013369 | A | 20050621 | BR 2003-13369 | 20030730 |
| CN 1678592 | A | 20051005 | CN 2003-820742 | 20030730 |
| JP 2006500343 | T | 20060105 | JP 2004-526225 | 20030730 |
| MX 2005PA01288 | A | 20050908 | MX 2005-PA1288 | 20050201 |
| IN 2005KN00293 | A | 20051125 | IN 2005-KN293 | 20050228 |
| PRIORITY APPLN. INFO.: | | | US 2002-399702P | P 20020801 |
| | | | WO 2003-US23791 | W 20030730 |

OTHER SOURCE(S): MARPAT 140:181460

ED Entered STN: 13 Feb 2004

GI



AB Title compds. I [wherein R1 = independently halogen, (halo)alkyl, alkoxy, hydroxyalkyl, amino, nitro, cyano; R2, R3 = independently H, (cyclo)alkyl, haloalkyl, hydroxyalkyl, or R2 and R3 together with the nitrogen atom to which they are attached form an (un)substituted heterocyclic ring; R4 = (un)substituted phenoxyphenyl, phenylthiophenyl, phenylaminophenyl, benzylphenyl, etc.; n = 0-3; p = 2-4; X = N, NH, S; Y = O, S; and pharmaceutically acceptable salts or solvates thereof] were prepared as sodium channel blockers. For example, reaction of 2-(piperidin-1-yl)ethylamine with

2-nitrobenzoyl chloride, followed by 10% Pd/C-catalyzed reduction and condensation with 3,3-diphenylpropenal, gave II. I were formulated as tablets and i.v. solns. Selected compds. of the invention inhibited sodium channel activity with Ki values ranging from 1 nM to 3960 nM. Thus, I and their pharmaceutical compns. are useful as sodium channel blockers for the treatment of neuronal damage following global or focal ischemia, neurodegenerative conditions, such as amyotrophic lateral sclerosis (ALS), acute or chronic pain, neuropathic pain, surgical pain, tinnitus, convulsions, manic depression, arrhythmia and diabetic neuropathy (no data).

- IC ICM C07D239-91
- ICS C07D279-08; A61K031-517; A61K031-5415
- CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
- Section cross-reference(s): 1, 63
- ST quinazolinone piperidinylethyl prepn sodium channel blocker;
benzothiazinone piperidinylethyl prepn sodium channel blocker;
benzoheterocycle piperidinylethyl prepn antiischemic analgesics
antidepressant antiarrhythmics antitinnitus anticonvulsants
- IT Pain
(acute; preparation of piperidinylethyl quinazolinone and
benzothiazinone derivs. for use as sodium channel blockers)
- IT Nervous system, disease
(amyotrophic lateral sclerosis; preparation of piperidinylethyl
quinazolinone and benzothiazinone derivs. for use as sodium
channel blockers)
- IT Heart, disease
(arrhythmia; preparation of piperidinylethyl quinazolinone and
benzothiazinone derivs. for use as sodium channel blockers)
- IT Pain
(chronic; preparation of piperidinylethyl quinazolinone and
benzothiazinone derivs. for use as sodium channel blockers)
- IT Nerve, disease
Nervous system, disease
(degeneration; preparation of piperidinylethyl quinazolinone and
benzothiazinone derivs. for use as sodium channel blockers)
- IT Mental and behavioral disorders
(depression, manic; preparation of piperidinylethyl quinazolinone
and benzothiazinone derivs. for use as sodium channel blockers)
- IT Nerve, disease
(diabetic neuropathy; preparation of piperidinylethyl quinazolinone
and benzothiazinone derivs. for use as sodium channel blockers)
- IT Anesthetics
(local; preparation of piperidinylethyl quinazolinone and
benzothiazinone derivs. for use as sodium channel blockers)
- IT Antidepressants
(manic; preparation of piperidinylethyl quinazolinone and
benzothiazinone derivs. for use as sodium channel blockers)
- IT Nerve, disease
Pain
(neuralgia; preparation of piperidinylethyl quinazolinone and
benzothiazinone derivs. for use as sodium channel blockers)
- IT Cytoprotective agents
Nervous system agents
(neuroprotective agents; preparation of piperidinylethyl
quinazolinone and benzothiazinone derivs. for use as sodium
channel blockers)
- IT Analgesics
Anti-ischemic agents
Antiarrhythmics
Anticonvulsants
Convulsion

Human
Ischemia
Sodium channel blockers
Tinnitus

- (preparation of piperidinylethyl quinazolinone and benzothiazinone derivs. for use as sodium channel blockers)
- IT Drug delivery systems
(sols., i.v.; preparation of piperidinylethyl quinazolinone and benzothiazinone derivs. for use as sodium channel blockers)
- IT Pain
(surgical; preparation of piperidinylethyl quinazolinone and benzothiazinone derivs. for use as sodium channel blockers)
- IT Drug delivery systems
(tablets; preparation of piperidinylethyl quinazolinone and benzothiazinone derivs. for use as sodium channel blockers)
- IT 658044-66-7P 658044-67-8P 658044-68-9P 658044-69-0P 658044-70-3P
658044-71-4P 658044-72-5P 658044-73-6P 658044-74-7P 658044-75-8P
658044-77-0P 658044-79-2P 658044-81-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of piperidinylethyl quinazolinone and benzothiazinone derivs. for use as sodium channel blockers)
- IT 84-58-2, 2,3-Dichloro-5,6-dicyano-1,4-benzoquinone 147-93-3,
2-Mercaptobenzoic acid 610-14-0, 2-Nitrobenzoyl chloride 1074-01-7,
Benzoic acid, o-mercaptothio- 1210-39-5 1700-37-4,
3-Benzyloxybenzaldehyde 27578-60-5, 2-(Piperidin-1-yl)ethylamine
69770-23-6 78725-46-9 79124-76-8, 3-(3,4-Dichlorophenoxy)benzaldehyde
137736-06-2, 4-(4-Fluorophenoxy)benzaldehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of piperidinylethyl quinazolinone and benzothiazinone derivs. for use as sodium channel blockers)

L56 ANSWER 5 OF 12 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:635488 HCAPLUS Full-text

TITLE: A facile thermal conversion of arylcyanoguanidines to 2,4-diaminoquinazolines

AUTHOR(S): Shao, Bin; Huang, Jin-cheng

CORPORATE SOURCE: Computational, Combinatorial and Medicinal Chemistry department, Purdue Pharma, L.P., Cranbury, NJ, 08512, USA

SOURCE: Abstracts of Papers, 226th ACS National Meeting, New York, NY, United States, September 7-11, 2003 (2003), ORGN-401. American Chemical Society: Washington, D. C.
CODEN: 69EKY9

DOCUMENT TYPE: Conference; Meeting Abstract

LANGUAGE: English

ED Entered STN: 15 Aug 2003

AB Herein we would like to report a facile, thermally induced conversion of arylcyanoguanidines to 2,4-diaminoquinazolines. Diphenoxycyanimidate was sequentially treated with anilines of diverse electronic properties followed by secondary amines to form stable intermediates of type B, which upon heating at 120°C in p-xylene in the absence of catalyst cyclize to give high yields of 2,4-diaminoquinazolines (Scheme 1).

L56 ANSWER 6 OF 12 HCAPLUS COPYRIGHT 2008 ACS on STN

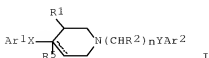
ACCESSION NUMBER: 1997:503392 HCAPLUS Full-text

DOCUMENT NUMBER: 127:149079

ORIGINAL REFERENCE NO.: 127:28801a,28804a
 TITLE: Preparation of 4-substituted piperidine analogs and their use as subtype selective NMDA receptor antagonists
 INVENTOR(S): Bigge, Christopher F.; Cai, Sui Xiong; Weber, Eckard; Woodward, Richard; Keana, John F. W.; Lan, Nancy C.; Guzikowski, Anthony P.; Zhou, Zhang-Lin; Yeun, Po-Wai
 PATENT ASSIGNEE(S): Warner-Lambert Company, USA; Cocensys, Inc.; Bigge, Christopher F.; Cai, Sui Xiong; Weber, Eckard; Woodward, Richard; Keana, John F. W.; Lan, Nancy C.; Guzikowski, Anthony P.; et al.
 SOURCE: PCT Int. Appl., 280 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|------------|
| WO 9723216 | A1 | 19970703 | WO 1996-US20872 | 19961220 |
| W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN | | | | |
| RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG | | | | |
| ZA 9610745 | A | 19970624 | ZA 1996-10745 | 19961219 |
| CA 2240275 | A1 | 19970703 | CA 1996-2240275 | 19961220 |
| AU 9716899 | A | 19970717 | AU 1997-16899 | 19961220 |
| AU 717185 | B2 | 20000316 | | |
| EP 869792 | A2 | 19981014 | EP 1996-945682 | 19961220 |
| EP 869792 | B1 | 20050309 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |
| BR 9612686 | A | 19990720 | BR 1996-12686 | 19961220 |
| HU 9901296 | A2 | 19990830 | HU 1999-1296 | 19961220 |
| HU 9901296 | A3 | 20010129 | | |
| JP 2000500773 | T | 20000125 | JP 1997-523887 | 19961220 |
| NZ 330624 | A | 20000327 | NZ 1996-330624 | 19961220 |
| IL 125061 | A | 20040512 | IL 1996-125061 | 19961220 |
| AT 290380 | T | 20050315 | AT 1996-945682 | 19961220 |
| NO 9802870 | A | 19980824 | NO 1998-2870 | 19980619 |
| NO 314580 | B1 | 20030414 | | |
| BG 63380 | B1 | 20011231 | BG 1998-102562 | 19980619 |
| US 6124323 | A | 20000926 | US 1998-91598 | 19980916 |
| PRIORITY APPLN. INFO.: | | | US 1995-9184P | P 19951222 |
| | | | WO 1996-US20872 | W 19961220 |

OTHER SOURCE(S): MARPAT 127:149079
 ED Entered SIN: 09 Aug 1997
 GI



AB 4-Substituted piperidine analogs I [Ar1, Ar2 = aryl, heteroaryl; X = (CHR3)m, O, S, NR4; R3 = H, OH, alkyl; R4 = H, alkyl; m = 0, 1, 2; R1 = H, OH, alkyl; n = 0-4; Y = O, S, NR4, or a single bond; R5 = H, OH; the dotted bond is a single or double bond] were prepared as selective active antagonists of N-methyl-D-aspartate (NMDA) receptor subtypes. E.g., reaction of 4-benzylpiperidine and 1-bromo-2-phenoxyethane gave 4-benzyl-1-(2-phenoxyethyl)piperidine. Data show that I exhibit selectivity for 2B subtype receptors compared to 2A and 2C subtype receptors. Many of the compds. are active as anticonvulsants. I also show significant protection from ischemia.

IC ICM A61K031-445
ICS C07D211-14

CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 63

IT 88-75-5, 2-Nitrophenol 90-15-3, 1-Naphthyl alcohol 98-17-9, 3-(Trifluoromethyl)phenol 100-02-7, reactions 100-39-0, Benzyl bromide 100-48-1, 4-Cyanopyridine 100-61-8, N-Methylaniline, reactions 100-83-4, 3-Hydroxybenzaldehyde 103-16-2, 4-Benzoyloxyphenol 103-63-9, (2-Bromoethyl)benzene 104-81-4, 4-Methylbenzyl bromide 104-82-5, 4-Methylbenzyl chloride 106-47-8, 4-Chloroaniline, reactions 106-89-8, reactions 108-95-2, Phenol, reactions 108-98-5, Thiophenol, reactions 109-04-6, 2-Bromopyridine 148-24-3, 8-Hydroxyquinoline, reactions 332-48-9 367-12-4, 2-Fluorophenol 371-40-4, 4-Fluoroaniline 371-41-5, 4-Fluorophenol 402-49-3, 4-(Trifluoromethyl)benzyl bromide 452-74-4 459-46-1, 4-Fluorobenzyl bromide 462-06-6, Fluorobenzene 491-36-1, 4-Hydroxyquinazoline 498-94-2, Isonipecotic acid 501-97-3 533-31-3, Sesamol 536-60-7, 4-Isopropylbenzyl alcohol 554-84-7, 3-Nitrophenol 580-13-2, 2-Bromonaphthalene 580-16-5, 6-Hydroxyquinoline 588-63-6 589-10-6, 1-Bromo-2-phenoxyethane 603-35-0, Triphenylphosphine, reactions 603-85-0, 2-Amino-3-nitrophenol 610-81-1, 4-Amino-3-nitrophenol 621-37-4, 3-Hydroxyphenylacetic acid 621-87-4, Phenoxyacetone 622-08-2, 2-Benzoyloxyethanol 637-59-2, 1-Bromo-3-phenylpropane 637-89-8, 4-Hydroxythiophenol 768-56-9, 4-Phenyl-1-butene 771-99-3, 4-Phenylpiperidine 876-02-8 877-65-6, 4-tert-Butylbenzyl alcohol 1072-85-1 1129-78-8 1190-22-3, 1,3-Dichlorobutane 1200-03-9, 4-Phenoxybutyl bromide 1476-11-5 1936-57-8, 4-Methylaminophenol sulfate 2033-76-3 2041-17-0 2042-14-0, 4-Methyl-3-nitrophenol 2116-65-6, 4-Benzylpyridine 3245-45-2 3351-59-5 3384-04-1, 3-Phenoxypropyl chloride 3612-20-2 4409-11-4 4463-59-6 4783-86-2, 4-Phenoxypyridine 4830-93-7, 1-Chloro-4-phenylbutane 6748-48-7 6940-76-7, 1-Chloro-3-iodopropane 10315-03-4 13288-06-7 13633-25-5, 1-Bromo-4-phenylbutane 17138-28-2, Ethyl 4-Hydroxyphenylacetate 18800-34-5 18800-37-8 19524-06-2, 4-Bromopyridine hydrochloride 20662-53-7 22009-38-7, 7-Hydroxy-1-tetralone 22921-76-2 31252-42-3, 4-Benzylpiperidine 31406-95-8 33349-49-4 34361-23-4 36938-76-8 36968-94-2 37142-39-5 37581-26-3 39512-49-7 39546-32-2, Isonipecotamide 40807-61-2 41979-39-9, 4-Piperidone hydrochloride 43224-81-3, 2-Phenoxyethyl tosylate 50562-02-2 51135-96-7, 4-Benzyl-4-hydroxypiperidine 51304-58-6 51974-48-2 57825-30-6, 4-Ethylbenzyl bromide 59216-77-2 70743-66-7 79098-85-4 85118-00-9, 2,6-Difluorobenzyl bromide 85118-01-0, 3,4-Difluorobenzyl bromide 92822-01-0 92822-03-2 107332-83-2 118495-07-1 141498-79-5 152604-19-8 177172-38-2 192182-59-5 192872-94-9 192872-97-2 193220-23-4 193356-97-7 193356-99-9 193357-07-2 193357-11-8 193357-17-4 193357-21-0 193357-26-5 193357-31-2 193357-34-5 193357-36-7 193357-39-0 193357-42-5 193357-43-6 193357-44-7

RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of piperidine derivs. and their use as subtype selective NMDA
 receptor antagonists)

=> d ibib ab hitstr 7-9

YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS, USPATFULL, BIOSIS, SCISEARCH' -
 CONTINUE? (Y)/N:y

L56 ANSWER 7 OF 12 USPATFULL on SIN DUPLICATE 3
 ACCESSION NUMBER: 2002:268763 USPATFULL Full-text
 TITLE: Substituted quinazolines and analogs and use thereof
 INVENTOR(S): Upasani, Ravi, San Jose, CA, United States
Cai, Guo X., San Diego, CA, United States
Lau, Nancy C., S. Pasadena, CA, United States
Wang, Yan, San Diego, CA, United States
Field, George, Danville, CA, United States
Flick, David B., Newport Beach, CA, United States
 STATES
 PATENT ASSIGNEE(S): Euro-Celtique S.A., Luxembourg,
 LUXEMBOURG (non-U.S. corporation)

| | NUMBER | KIND | DATE |
|-----------------------|--|------|--------------|
| PATENT INFORMATION: | US 6465472 | B1 | 20021015 |
| APPLICATION INFO.: | US 2000-654839 | | 20000901 (9) |
| RELATED APPLN. INFO.: | Continuation of Ser. No. WO 1999-US4609, filed on 2 Mar 1999 | | |

| | NUMBER | DATE |
|-----------------------|---|---------------|
| PRIORITY INFORMATION: | US 1998-76451P | 19980302 (60) |
| DOCUMENT TYPE: | Utility | |
| FILE SEGMENT: | GRANTED | |
| PRIMARY EXAMINER: | Shah, Mukund J. | |
| ASSISTANT EXAMINER: | Liu, Hong | |
| LEGAL REPRESENTATIVE: | Sterne, Kessler, Goldstein & Fox P.L.L.C. | |
| NUMBER OF CLAIMS: | 16 | |
| EXEMPLARY CLAIM: | 1 | |
| NUMBER OF DRAWINGS: | 0 Drawing Figure(s); 0 Drawing Page(s) | |
| LINE COUNT: | 2866 | |

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

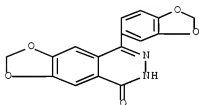
AB The invention relates to novel quinazolines and heterocycles which are antagonists or positive modulators of AMPA receptors, and the use thereof for treating, preventing or ameliorating neuronal loss associated with stroke, global and focal ischemia, CNS trauma, hypoglycemia and surgery, as well as treating or ameliorating neurodegenerative diseases including Alzheimer's disease, amyotrophic lateral sclerosis, Huntington's disease, Parkinson's disease and Down's syndrome, treating, preventing or ameliorating the adverse consequences of the overstimulation of the excitatory amino acids, treating, preventing or ameliorating anxiety, psychosis, convulsions, chronic pain, glaucoma, retinitis, urinary incontinence, muscular spasm and inducing anesthesia, as well as for treating or ameliorating the adverse consequences of excitatory amino acid deficiency such as schizophrenia, myoclonus. Alzheimer's disease and malnutrition and neural maldevelopment, and as cognition and learning enhancers.

IT 243134-66-9P

(target compound; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)

RN 243134-66-9 USPATFULL

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(1,3-benzodioxol-5-yl)- (CA INDEX NAME)

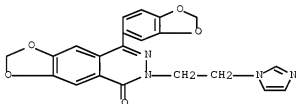
IT 243134-67-0P 243134-66-1P 243134-69-2P

243134-70-5P 243134-71-6P 243134-72-7P

(target compound; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)

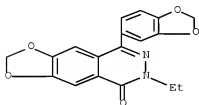
RN 243134-67-0 USPATFULL

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-[2-(1H-imidazol-1-yl)ethyl]- (CA INDEX NAME)

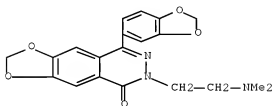


RN 243134-68-1 USPATFULL

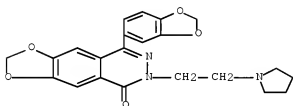
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(1,3-benzodioxol-5-yl)-6-ethyl- (CA INDEX NAME)



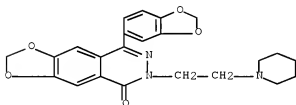
RN 243134-69-2 USPATFULL

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one,
8-(1,3-benzodioxol-5-yl)-6-[2-(dimethylamino)ethyl]- (CA INDEX NAME)

RN 243134-70-5 USPATFULL

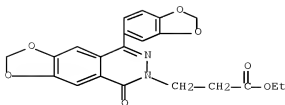
CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one,
8-(1,3-benzodioxol-5-yl)-6-[2-(1-pyrrolidinyl)ethyl]- (CA INDEX NAME)

RN 243134-71-6 USPATFULL

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one,
8-(1,3-benzodioxol-5-yl)-6-[2-(1-piperidiny)ethyl]- (CA INDEX NAME)

RN 243134-72-7 USPATFULL

CN 1,3-Dioxolo[4,5-g]phthalazine-6(5H)-propanoic acid,
8-(1,3-benzodioxol-5-yl)-5-oxo-, ethyl ester (CA INDEX NAME)



L56 ANSWER 8 OF 12 USPATFULL on SIN

ACCESSION NUMBER: 2004:209865 USPATFULL Full-text
 TITLE: Substituted quinazolines and analogs and the use thereof

INVENTOR(S): Dasani, Ravi, San Jose, CA, UNITED STATES
Cai, Sui X., San Diego, CA, UNITED STATES
Lan, Nancy C., Pasadena, CA, UNITED STATES
Wang, Yan, San Diego, CA, UNITED STATES
Field, George, Danville, CA, UNITED STATES
Pick, David B., Mission Viejo, CA, UNITED STATES

PATENT ASSIGNEE(S): Euro-Celtique, S.A. (U.S. corporation)

| | NUMBER | KIND | DATE |
|-----------------------|--|------|---------------|
| PATENT INFORMATION: | US 20040162299 | A1 | 20040819 |
| APPLICATION INFO.: | US 2004-772445 | A1 | 20040206 (10) |
| RELATED APPLN. INFO.: | Division of Ser. No. US 2002-219755, filed on 16 Aug 2002, PENDING Division of Ser. No. US 2000-654839, filed on 1 Sep 2000, GRANTED, Pat. No. US 6465472 Continuation of Ser. No. WO 1999-US4609, filed on 2 Mar 1999, PENDING | | |

| | NUMBER | DATE |
|-----------------------|--|---------------|
| PRIORITY INFORMATION: | US 1998-76451P | 19980302 (60) |
| DOCUMENT TYPE: | Utility | |
| FILE SEGMENT: | APPLICATION | |
| LEGAL REPRESENTATIVE: | STERNE, KESSLER, GOLDSTEIN & FOX PLLC, 1100 NEW YORK AVENUE, N.W., WASHINGTON, DC, 20005 | |
| NUMBER OF CLAIMS: | 33 | |
| EXEMPLARY CLAIM: | 1 | |
| LINE COUNT: | 3033 | |

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The invention relates to novel quinazolines and heterocycles which are antagonists or positive modulators of AMPA receptors, and the use thereof for treating, preventing or ameliorating neuronal loss associated with stroke, global and focal ischemia, CNS trauma, hypoglycemia and surgery, as well as treating or ameliorating neurodegenerative diseases including Alzheimer's disease, amyotrophic lateral sclerosis, Huntington's disease, Parkinson's disease and Down's syndrome, treating, preventing or ameliorating the adverse consequences of the overstimulation of the excitatory amino acids, treating, preventing or ameliorating anxiety, psychosis, convulsions, chronic pain, glaucoma, retinitis, urinary incontinence, muscular spasm and inducing anesthesia, as well as for treating or ameliorating the adverse consequences of excitatory amino acid

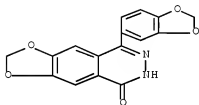
deficiency such as schizophrenia, myoclonus, Alzheimer's disease and malnutrition and neural maldevelopment, and as cognition and learning enhancers.

IT 243134-66-9P

(target compound; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)

RN 243134-66-9 USPATFULL

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(1,3-benzodioxol-5-yl)- (CA INDEX NAME)



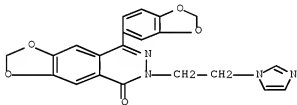
IT 243134-67-0P 243134-68-1P 243134-69-2P

243134-70-5P 243134-71-6P 243134-72-7P

(target compound; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)

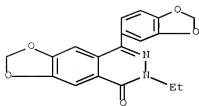
RN 243134-67-0 USPATFULL

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(1,3-benzodioxol-5-yl)-6-[2-(1H-imidazol-1-yl)ethyl]- (CA INDEX NAME)



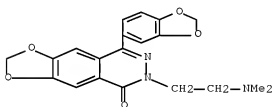
RN 243134-68-1 USPATFULL

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(1,3-benzodioxol-5-yl)-6-ethyl- (CA INDEX NAME)



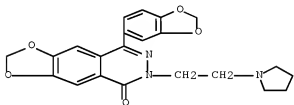
RN 243134-69-2 USPATFULL

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one,
8-(1,3-benzodioxol-5-yl)-6-[2-(dimethylamino)ethyl]- (CA INDEX NAME)



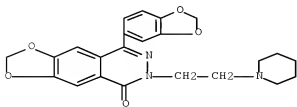
RN 243134-70-5 USPATFULL

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one,
8-(1,3-benzodioxol-5-yl)-6-[2-(1-pyrrolidinyl)ethyl]- (CA INDEX NAME)

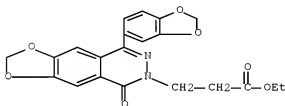


RN 243134-71-6 USPATFULL

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one,
8-(1,3-benzodioxol-5-yl)-6-[2-(1-piperidinyl)ethyl]- (CA INDEX NAME)



RN 243134-72-7 USPATFULL
 CN 1,3-Dioxolo[4,5-g]phthalazine-6(5H)-propanoic acid,
 8-(1,3-benzodioxol-5-yl)-5-oxo-, ethyl ester (CA INDEX NAME)



L56 ANSWER 9 OF 12 USPATFULL on SIN

ACCESSION NUMBER: 2003:45776 USPATFULL Full-text
 TITLE: Substituted quinazolines and analogs and the use thereof
 INVENTOR(S): Upasani, Ravi, Sunnyvale, CA, UNITED STATES
Cai, Gui X., San Diego, CA, UNITED STATES
Lan, Nancy C., Altadena, CA, UNITED STATES
 PATENT ASSIGNEE(S): Euro-Celtique S.A. (U.S. corporation)

| | NUMBER | KIND | DATE |
|-----------------------|--|------|---------------|
| PATENT INFORMATION: | US 20030033089 | A1 | 20030213 |
| | US 6765006 | B2 | 20040720 |
| APPLICATION INFO.: | US 2002-219755 | A1 | 20020816 (10) |
| RELATED APPLN. INFO.: | Division of Ser. No. US 2000-654839, filed on 1 Sep 2000, GRANTED, Pat. No. US 6465472 Continuation of Ser. No. WO 1999-US4609, filed on 2 Mar 1999, PENDING | | |

| | NUMBER | DATE |
|-----------------------|--|---------------|
| PRIORITY INFORMATION: | US 1998-76451P | 19980302 (60) |
| DOCUMENT TYPE: | Utility | |
| FILE SEGMENT: | APPLICATION | |
| LEGAL REPRESENTATIVE: | STERNE, KESSLER, GOLDSTEIN & FOX PLLC, 1100 NEW YORK AVENUE, N.W., SUITE 600, WASHINGTON, DC, 20005-3934 | |
| NUMBER OF CLAIMS: | 33 | |
| EXEMPLARY CLAIM: | 1 | |
| LINE COUNT: | 3018 | |

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The invention relates to novel quinazolines and heterocycles which are antagonists or positive modulators of AMPA receptors, and the use thereof for treating, preventing or ameliorating neuronal loss associated with stroke, global and focal ischemia, CNS trauma, hypoglycemia and surgery, as well as treating or ameliorating neurodegenerative diseases including Alzheimer's disease, amyotrophic lateral sclerosis, Huntington's disease, Parkinson's disease and Down's syndrome, treating, preventing or ameliorating the adverse consequences of the overstimulation of the excitatory amino acids, treating, preventing or ameliorating anxiety, psychosis, convulsions, chronic pain, glaucoma, retinitis, urinary incontinence, muscular spasm and inducing anesthesia, as well as for

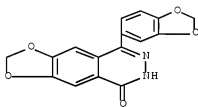
treating or ameliorating the adverse consequences of excitatory amino acid deficiency such as schizophrenia, myoclonus, Alzheimer's disease and malnutrition and neural maldevelopment, and as cognition and learning enhancers.

IT 243134-66-9P

(target compound; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)

RN 243134-66-9 USPATFULL

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(1,3-benzodioxol-5-yl)- (CA INDEX NAME)



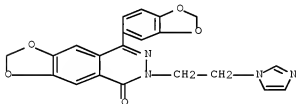
IT 243134-67-0P 243134-68-1P 243134-69-2P

243134-70-5P 243134-71-6P 243134-72-7P

(target compound; preparation of substituted quinazolines and heterocyclic analogs as antagonists or pos. modulators of AMPA receptors for treatment of global ischemia, amyotrophic lateral sclerosis, acute or chronic pain, or schizophrenia)

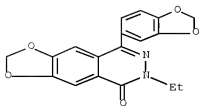
RN 243134-67-0 USPATFULL

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(1,3-benzodioxol-5-yl)-6-[2-(1H-imidazol-1-yl)ethyl]- (CA INDEX NAME)



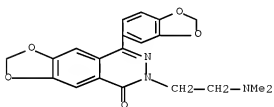
RN 243134-68-1 USPATFULL

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one, 8-(1,3-benzodioxol-5-yl)-6-ethyl- (CA INDEX NAME)



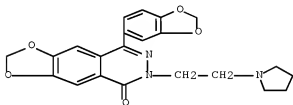
RN 243134-69-2 USPATFULL

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one,
8-(1,3-benzodioxol-5-yl)-6-[2-(dimethylamino)ethyl]- (CA INDEX NAME)



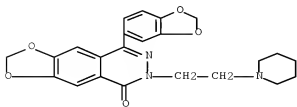
RN 243134-70-5 USPATFULL

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one,
8-(1,3-benzodioxol-5-yl)-6-[2-(1-pyrrolidinyl)ethyl]- (CA INDEX NAME)

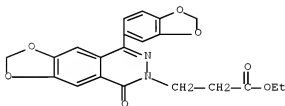


RN 243134-71-6 USPATFULL

CN 1,3-Dioxolo[4,5-g]phthalazin-5(6H)-one,
8-(1,3-benzodioxol-5-yl)-6-[2-(1-piperidinyl)ethyl]- (CA INDEX NAME)



RN 243134-72-7 USPATFULL
 CN 1,3-Dioxolo[4,5-g]phthalazine-6(5H)-propanoic acid,
 8-(1,3-benzodioxol-5-yl)-5-oxo-, ethyl ester (CA INDEX NAME)



=> d ibib ed ab ind 10-12

YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS, USPATFULL, BIOSIS, SCISEARCH' -
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L56 ANSWER 10 OF 12 BIOSIS COPYRIGHT (c) 2008 The Thomson Corporation on
 STN DUPLICATE 1

ACCESSION NUMBER: 2005:473259 BIOSIS Full-text
 DOCUMENT NUMBER: PREV200510263078

TITLE: Quinazolinones and benzothiazinones as novel
 sodium channel blockers.

AUTHOR(S): Victory, Sam F. [Reprint Author]; Sun, Qun; Limberis, Jim;
 Kyle, Donald J.

CORPORATE SOURCE: Purdue Pharma, Discovery Res, Cranbury,
 NJ 08512 USA
 sam.victory@pharma.com

SOURCE: Abstracts of Papers American Chemical Society, (AUG 22
 2004) Vol. 228, No. Part 1, pp. U920.
 Meeting Info.: Meeting of the Division of Chemical
 Toxicology of the American-Chemical-Society held at the
 228th National Meeting of the American-Chemical-Society.
 Philadelphia, PA, USA. August 22 -26, 2004. Amer Chem Soc,
 Div Chem Toxicol.
 CODEN: ACSRAL. ISSN: 0065-7727.

DOCUMENT TYPE: Conference; (Meeting)
 Conference; Abstract; (Meeting Abstract)

LANGUAGE: English

ENTRY DATE: Entered STN: 16 Nov 2005
 Last Updated on STN: 16 Nov 2005

ED Entered STN: 16 Nov 2005
 Last Updated on STN: 16 Nov 2005

CC General biology - Symposia, transactions and proceedings 00520
 Biophysics - Membrane phenomena 10508
 Pathology - Therapy 12512
 Nervous system - Physiology and biochemistry 20504
 Nervous system - Pathology 20506
 Pharmacology - General 22002
 Pharmacology - Neuropharmacology 22024

IT Major Concepts
 Pharmacology; Nervous System (Neural Coordination)

IT Diseases
 neuropathic pain: nervous system disease, drug therapy
 Pain (MeSH)

IT Chemicals & Biochemicals
 sodium channel; V102862: analgesic-drug, semicarbazone moiety;
sodium channel blockers: analgesic-drug, thiazolidinone ring,
hydrophic aryl ether moiety, piperidinylethylamine moiety,
quinazolin-4(3H)-one core ring system, 2,3-dihydro-benzothiazin-4-one
core ring system

IT Miscellaneous Descriptors
 structure-activity relationship

L56 ANSWER 11 OF 12 BIOSIS COPYRIGHT (c) 2008 The Thomson Corporation on
 STN

ACCESSION NUMBER: 2004:332648 BIOSIS Full-text

DOCUMENT NUMBER: PREV200400337520

TITLE: Substituted quinazolines and analogs and the use
 thereof.

AUTHOR(S): Upasani, Ravi [Inventor, Reprint Author];
Cai, Sui X. [Inventor]

CORPORATE SOURCE: Sunnyvale, CA, USA

ASSIGNEE: Euro-Celtique S.A.,
 Luxembourg

PATENT INFORMATION: US 6765006 20040720

SOURCE: Official Gazette of the United States Patent and Trademark
 Office Patents, (July 20 2004) Vol. 1284, No. 3.
<http://www.uspto.gov/web/menu/patdata.html>. e-file.
 ISSN: 0098-1133 (ISSN print).

DOCUMENT TYPE: Patent

LANGUAGE: English

ENTRY DATE: Entered STN: 4 Aug 2004
 Last Updated on STN: 4 Aug 2004

ED Entered STN: 4 Aug 2004
 Last Updated on STN: 4 Aug 2004

AB The invention relates to novel quinazolines and heterocycles which are
 antagonists or positive modulators of AMPA receptors, and the use thereof for
 treating, preventing or ameliorating neuronal loss associated with stroke,
 global and focal ischemia, CNS trauma, hypoglycemia and surgery, as well as
 treating or ameliorating neurodegenerative diseases including Alzheimer's
 disease, amyotrophic lateral sclerosis, Huntington's disease, Parkinson's
 disease and Down's syndrome, treating, preventing or ameliorating the adverse
 consequences of the overstimulation of the excitatory amino acids, treating,
 preventing or ameliorating anxiety, psychosis, convulsions, chronic pain,
 glaucoma, retinitis, urinary incontinence, muscular spasm and inducing
 anesthesia, as well as for treating or ameliorating the adverse consequences
 of excitatory amino acid deficiency such as schizophrenia, myoclonus,
 Alzheimer's disease and malnutrition and neural maldevelopment, and as
 cognition and learning enhancers.

NCL 514232800

CC Pathology - Therapy 12512
 Urinary system - Pathology 15506
 Sense organs - Pathology 20006
 Nervous system - Pathology 20506
 Pharmacology - General 22002
 Pharmacology - Neuropharmacology 22024
 Pharmacology - Psychopharmacology 22026
 Pharmacology - Sense organs, associated structures and functions 22031

IT Major Concepts

Pharmacology

IT Diseases
anxiety: behavioral and mental disorders, drug therapy
Anxiety (MeSH)

IT Diseases
glaucoma: eye disease, drug therapy
Glaucoma (MeSH)

IT Diseases
malnutrition: nutritional disease, drug therapy
Nutrition Disorders (MeSH)

IT Diseases
neurological diseases: nervous system disease, drug therapy

IT Diseases
psychosis: behavioral and mental disorders, drug therapy
Psychotic Disorders (MeSH)

IT Diseases
retinitis: eye disease, drug therapy
Retinitis (MeSH)

IT Diseases
schizophrenia: behavioral and mental disorders, drug therapy
Schizophrenia (MeSH)

IT Diseases
urinary incontinence: urologic disease, drug therapy
Urinary Incontinence (MeSH)

IT Chemicals & Biochemicals
substituted quinazolines: anticonvulsant-drug,
antiglaucoma-drug, antiparkinsonian-drug, antipsychotic-drug, general
anesthetic-drug, neuroprotectant-drug, nootropic-drug, ophthalmic-drug,
AMPA receptor antagonists, analogs

RN 253-82-7D (substituted quinazolines)

L56 ANSWER 12 OF 12 SCISEARCH COPYRIGHT (c) 2008 The Thomson Corporation on
STN

ACCESSION NUMBER: 2004:180442 SCISEARCH Full-text

THE GENUINE ARTICLE: 751JG

TITLE: Facile thermal conversion of arylcyanoguanidines to 2,4-
diaminoquinazolines.

AUTHOR: Shao B (Reprint); Huang J C

CORPORATE SOURCE: Purdue Pharma, Computat Combinatorial
& Med Chem Dept, LP, Cranbury, NJ 08512 USA

COUNTRY OF AUTHOR: USA

SOURCE: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, (SEP
2003) Vol. 226, Part 2, pp. U180-U180. MA 401-ORGN.
ISSN: 0065-7727.

PUBLISHER: AMER CHEMICAL SOC, 1155 16TH ST, NW, WASHINGTON, DC 20036
USA.

DOCUMENT TYPE: Conference; Journal

LANGUAGE: English

REFERENCE COUNT: 0

ENTRY DATE: Entered STN: 5 Mar 2004
Last Updated on STN: 5 Mar 2004

ED Entered STN: 5 Mar 2004
Last Updated on STN: 5 Mar 2004

CC CHEMISTRY, MULTIDISCIPLINARY

=> file stnguide

FILE 'STNGUIDE' ENTERED AT 16:01:23 ON 04 DEC 2008
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

10/772,445

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Nov 21, 2008 (20081121/UP).

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(FILE 'HOME' ENTERED AT 13:48:16 ON 04 DEC 2008)

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E US2004-772445/APPS

L1 FILE 'HCAPLUS' ENTERED AT 13:48:53 ON 04 DEC 2008
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L2 FILE 'WPIX' ENTERED AT 13:49:03 ON 04 DEC 2008
1 SEA SPE=ON ABB=ON PLU=ON US2004-772445/APPS

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FILE 'HCAPLUS' ENTERED AT 13:49:41 ON 04 DEC 2008
D IBIB ED ABS IND L1

FILE 'STNGUIDE' ENTERED AT 13:49:48 ON 04 DEC 2008
D QUE L2

FILE 'WPIX' ENTERED AT 13:50:15 ON 04 DEC 2008
D IALL CODE L2

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L4 FILE 'REGISTRY' ENTERED AT 13:50:34 ON 04 DEC 2008
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L5 7 SEA SPE=ON ABB=ON PLU=ON L4 AND N2C4/ESS
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L6 FILE 'LREGISTRY' ENTERED AT 13:51:47 ON 04 DEC 2008
STR

L7 FILE 'REGISTRY' ENTERED AT 13:54:29 ON 04 DEC 2008
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D QUE STAT

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L8 STR L***

L9 FILE 'REGISTRY' ENTERED AT 13:56:40 ON 04 DEC 2008
0 SEA SSS SAM L8

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D QUE STAT

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 D QUE STAT
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 D QUE STAT
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 L17 ANALYZE PLU=ON L15 1- LC : 8 TERMS
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 FILE 'ZCAPLUS' ENTERED AT 15:27:13 ON 04 DEC 2008
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 L20 QUE SPE=ON ABB=ON PLU=ON CAI, S?/AU
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 L22 QUE SPE=ON ABB=ON PLU=ON WANG, Y?/AU
 L23 QUE SPE=ON ABB=ON PLU=ON FIELD, G?/AU
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 L25 QUE SPE=ON ABB=ON PLU=ON (COCENSYS OR (PURDUE(1W)PHARMA) OR
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FILE 'STNGUIDE' ENTERED AT 15:30:40 ON 04 DEC 2008

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 OR L23 OR L24 OR L25)
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 OR L23 OR L24 OR L25)
 L34 6 SEA SPE=ON ABB=ON PLU=ON L32 NOT L33

FILE 'STNGUIDE' ENTERED AT 15:32:46 ON 04 DEC 2008

FILE 'CAOLD' ENTERED AT 15:33:04 ON 04 DEC 2008
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FILE 'HCAPLUS' ENTERED AT 15:33:29 ON 04 DEC 2008
 L36 2 SEA SPE=ON ABB=ON PLU=ON CA52:15486I/OREF

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 D QUE STAT
 L39 33 SEA SSS FUL L13

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 L41 4 SEA SSS FUL L13 (8 REACTIONS)
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 OR L23 OR L24 OR L25)
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 RA00N7/DCN OR RA00N8/DCN) OR L45/DCR
 L47 1 SEA SPE=ON ABB=ON PLU=ON L46 AND (L19 OR L20 OR L21 OR L22
 OR L23 OR L24 OR L25)

L48 1 SEA SPE=ON ABB=ON PLU=ON L47 OR L2
 L49 1 SEA SPE=ON ABB=ON PLU=ON L47 AND L2
 L50 1 SEA SPE=ON ABB=ON PLU=ON L47 OR L49
 L51 0 SEA SPE=ON ABB=ON PLU=ON L46 NOT L50

FILE 'STNGUIDE' ENTERED AT 15:38:55 ON 04 DEC 2008

FILE 'HCAPLUS, WPIX, MEDLINE, BIOSIS, EMBASE, PASCAL, CABA, CEABA-VTB, LIFESCI, BIOENG, BIOTECHNO, BIOTECHDS, DRUGU, DRUGB, VETU, VETB, SCISEARCH, CONFSCI, DISSABS, RDISCLOSURE' ENTERED AT 15:39:34 ON 04 DEC 2008

L52 164 SEA SPE=ON ABB=ON PLU=ON (L19 OR L20 OR L21 OR L22 OR L23
 OR L24 OR L25) AND ?QUINAZOLIN?/IT, TI, CC, CT, ST, STP
 D QUE
 L53 37 SEA SPE=ON ABB=ON PLU=ON L52 AND (L19 OR L23 OR L21 OR L24)
 L54 15 SEA SPE=ON ABB=ON PLU=ON L52 AND L25

FILE 'STNGUIDE' ENTERED AT 15:41:42 ON 04 DEC 2008

D QUE STAT L10
 D QUE STAT L15
 D QUE NOS L17
 D L17 1-
 D QUE NOS L31
 D QUE NOS L34
 D QUE NOS L35
 D QUE NOS L36
 D QUE NOS L37
 D QUE STAT L41
 D QUE NOS L43
 D QUE STAT L45
 D QUE NOS L51

FILE 'HCAPLUS, CASREACT, TOXCENTER, CAOLD, CHEMCATS, CHEMINFORMRX'
 ENTERED AT 15:45:19 ON 04 DEC 2008

L55 24 DUP REM L31 L34 L35 L36 L37 L43 L51 (8 DUPLICATES REMOVED)
 ANSWERS '1-16' FROM FILE HCAPLUS
 ANSWER '17' FROM FILE CAOLD
 ANSWERS '18-20' FROM FILE CHEMCATS
 ANSWERS '21-24' FROM FILE CHEMINFORMRX
 SAVE TEMP L55 JAI445MAIN/A

FILE 'STNGUIDE' ENTERED AT 15:45:37 ON 04 DEC 2008

FILE 'HCAPLUS, CAOLD, CHEMCATS, CHEMINFORMRX' ENTERED AT 15:46:11 ON 04
 DEC 2008

D IBIB ED ABS HITIND HITSTR 1-16

FILE 'STNGUIDE' ENTERED AT 15:46:19 ON 04 DEC 2008

FILE 'HCAPLUS, CAOLD, CHEMCATS, CHEMINFORMRX' ENTERED AT 15:49:10 ON 04
 DEC 2008

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FILE 'STNGUIDE' ENTERED AT 15:49:10 ON 04 DEC 2008

FILE 'HCAPLUS, CAOLD, CHEMCATS, CHEMINFORMRX' ENTERED AT 15:49:21 ON 04
 DEC 2008

D IDE 18-20

10/772,445

FILE 'STNGUIDE' ENTERED AT 15:49:22 ON 04 DEC 2008

FILE 'HCAPLUS, CAOLD, CHEMCATS, CHEMINFORMRX' ENTERED AT 15:49:47 ON 04
DEC 2008

D BIB AB HIT 21-24

FILE 'STNGUIDE' ENTERED AT 15:49:48 ON 04 DEC 2008

FILE 'BEILSTEIN' ENTERED AT 15:50:54 ON 04 DEC 2008

D QUE STAT L39

SAVE TEMP L39 JAI445BEIP/A

D IDE L39 1

D RX L39 1

D IDE L39 2

D RX L39 2

D IDE L39 3

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 D QUE NOS L33
 D QUE NOS L42
 D QUE L45
 D QUE NOS L50
 D QUE L54

FILE 'HCAPLUS, USPATFULL, WPIX, BIOSIS, EMBASE, DRUGU, SCISEARCH' ENTERED
 AT 15:58:57 ON 04 DEC 2008

L56 12 DUP REM L30 L33 L42 L50 L54 (8 DUPLICATES REMOVED)
 ANSWERS '1-6' FROM FILE HCAPLUS
 ANSWERS '7-9' FROM FILE USPATFULL
 ANSWERS '10-11' FROM FILE BIOSIS
 ANSWER '12' FROM FILE SCISEARCH
 SAVE TEMP L56 JAI445INV/A

FILE 'STNGUIDE' ENTERED AT 15:59:14 ON 04 DEC 2008

FILE 'HCAPLUS, USPATFULL, BIOSIS, SCISEARCH' ENTERED AT 15:59:34 ON 04 DEC 2008

D IBIB ED ABS HITIND HITSTR 1-6

FILE 'STNGUIDE' ENTERED AT 15:59:36 ON 04 DEC 2008

FILE 'HCAPLUS, USPATFULL, BIOSIS, SCISEARCH' ENTERED AT 16:00:01 ON 04 DEC 2008

D IBIB AB HITSTR 7-9

FILE 'STNGUIDE' ENTERED AT 16:00:10 ON 04 DEC 2008

FILE 'HCAPLUS, USPATFULL, BIOSIS, SCISEARCH' ENTERED AT 16:00:25 ON 04 DEC 2008

D IBIB ED AB IND 10-12

FILE 'STNGUIDE' ENTERED AT 16:00:25 ON 04 DEC 2008

FILE 'STNGUIDE' ENTERED AT 16:01:23 ON 04 DEC 2008

FILE HOME

FILE STNGUIDE
 FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Nov 21, 2008 (20081121/UP).

FILE ZCAPLUS

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FILE COVERS 1907 - 4 Dec 2008 VOL 149 ISS 23
FILE LAST UPDATED: 3 Dec 2008 (20081203/ED)

ZCAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE HCAPLUS

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FILE COVERS 1907 - 4 Dec 2008 VOL 149 ISS 23
FILE LAST UPDATED: 3 Dec 2008 (20081203/ED)

HCAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE WPIX

FILE LAST UPDATED: 28 NOV 2008 <20081128/UP>
MOST RECENT UPDATE: 200877 <200877/DW>

DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

>>> Now containing more than 1.2 million chemical structures in DCR <<<

>>> IPC Reform backfile reclassifications have been loaded to end of September 2008. No update date (UP) has been created for the reclassified documents, but they can be identified by 20060101/UPIC, and 20061231/UPIC, 20070601/UPIC, 20071001/UPIC, 20071130/UPIC, 20080401/UPIC, 20080701/UPIC and 20081001/UPIC.
ECLA reclassifications to mid August and US national classification

mid September 2008 have also been loaded. Update dates 20080401, 20080701 and 20081001/UPEC and /UPNC have been assigned to these. <<

FOR A COPY OF THE DERWENT WORLD PATENTS INDEX STN USER GUIDE,
PLEASE VISIT:
http://www.stn-international.de/training_center/patents/stn_guide.pdf

FOR DETAILS OF THE PATENTS COVERED IN CURRENT UPDATES, SEE
<http://scientific.thomsonreuters.com/support/patents/coverage/latestupdate>

EXPLORE DERWENT WORLD PATENTS INDEX IN STN ANAVIST, VERSION 2.0:
http://www.stn-international.com/DWPIAnaVist2_0608.html

>>> HELP for European Patent Classifications see HELP ECLA, HELP ICO <<<

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 2 DEC 2008 HIGHEST RN 1078799-92-4
DICTIONARY FILE UPDATES: 2 DEC 2008 HIGHEST RN 1078799-92-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

FILE LREGISTRY

LREGISTRY IS A STATIC LEARNING FILE

NEW CAS INFORMATION USE POLICIES, ENTER HELP USAGETERMS FOR DETAILS.

FILE USPATFULL

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 4 Dec 2008 (20081204/PD)
FILE LAST UPDATED: 4 Dec 2008 (20081204/ED)
HIGHEST GRANTED PATENT NUMBER: US7461407
HIGHEST APPLICATION PUBLICATION NUMBER: US20080301844
CA INDEXING IS CURRENT THROUGH 4 Dec 2008 (20081204/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 4 Dec 2008 (20081204/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Aug 2008
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Aug 2008

USPATFULL now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

FILE USPATOLD

FILE COVERS U.S. PATENTS 1790-1975
Produced using data provided by Univentio.

This database was created using Optical Character Recognition (OCR) technology. For this reason, some characters may be missing or mistranslated. In order to improve searchability and retrieval, CA indexing information has been added to the Title, Inventor, and Patent Assignee fields where possible. Please see HELP CASDATA for more information on the availability of CAS indexing in this database.

USPATOLD now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

FILE USPAT2

FILE COVERS 2001 TO PUBLICATION DATE: 4 Dec 2008 (20081204/PD)
 FILE LAST UPDATED: 4 Dec 2008 (20081204/ED)
 HIGHEST GRANTED PATENT NUMBER: US20080227788
 HIGHEST APPLICATION PUBLICATION NUMBER: US20080300718
 CA INDEXING IS CURRENT THROUGH 4 Dec 2008 (20081204/UPCA)
 ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 4 Dec 2008 (20081204/PD)
 REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2008
 USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2008

USPAT2 now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

FILE CASREACT

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FILE CONTENT:1840 - 29 Nov 2008 VOL 149 ISS 23

New CAS Information Use Policies, enter HELP USAGETERMS for details.

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*
*      CASREACT now has more than 15.3 million reactions      *
*
*
*****
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CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE TOXCENTER

FILE COVERS 1907 TO 2 Dec 2008 (20081202/ED)

The MEDLINE file segment has been updated with the National Library of Medicine's revised 2008 MeSH terms. See HELP RLOAD for details.

This file contains CAS Registry Numbers for easy and accurate substance

identification.

The BIOSIS segment of TOXCENTER has been augmented with 13,000 records from 1946 through 1968.

FILE CAOLD
FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

CAOLD will be discontinued and removed from associated database clusters.

- . November 22, 2008 - removed from database clusters
- . December 31, 2008 - removed from STN

Content previously available only in CAOLD is now available in CA/Caplus. To learn more about the options available for transferring saved search queries and answer sets to CA/Caplus, contact your STN Service Center.

FILE CHEMCATS

FILE LAST UPDATED 22 NOVEMBER 2008 (20081122/UP)

For details on recent updates in CHEMCATS, enter NEWS FILE at an arrow prompt. For the list of suppliers currently in the file, enter HELP SPA, HELP SPB, HELP SPC, HELP SPDH, HELP SPIN, HELP SPOQ, HELP SPRS, and HELP SPTZ. For the list of current catalogs, enter HELP CTA, HELP CTB, HELP CTC, HELP CTDH, HELP CTIL, HELP CTMN, HELP CTOQ, HELP CTRS, and HELP CTTZ.

This database is provided on an "as is" basis. Please consult the suppliers for current information regarding pricing, regional availability, available quantities, purities, etc. THERE ARE NO WARRANTIES OF ANY KIND, EITHER EXPRESSED OR IMPLIED. ACS is not liable for any loss of profit, goodwill or any other damages arising out of the use of this database.

CHEMCATS now contains more than 25 million records. See HELP CONTENT and NEWS FILE for details.

FILE BEILSTEIN
FILE LAST UPDATED ON April 1, 2008

FILE COVERS 1771 TO 2008.
FILE CONTAINS 10,322,806 SUBSTANCES

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For more detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

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* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. *
* FOR PRICE INFORMATION SEE HELP COST *
*****

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>>> Price change as of January 1st, 2008: Connect Time and Structure Search fees re-introduced. See NEWS and HELP COST <<<

FILE CHEMINFORMRX

FILE LAST UPDATED: 16 OCT 2008 <20081016/UP>

>>> CAS Registry Numbers are available for substances prior to 1995 <<<

FILE MEDLINE

FILE LAST UPDATED: 3 Dec 2008 (20081203/UP). FILE COVERS 1949 TO DATE.

MEDLINE has been updated with the National Library of Medicine's revised 2008 MeSH terms. See HELP RLOAD for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

See HELP RANGE before carrying out any RANGE search.

MEDLINE Accession Numbers (ANs) for records from 1950-1977 have been converted from 8 to 10 digits. Searches using an 8 or 10 digit AN will retrieve the same record. The 10-digit ANs can be expanded, searched, and displayed in all records from 1949 to the present.

FILE BIOSIS

FILE COVERS 1926 TO DATE.

CAS REGISTRY NUMBERS AND CHEMICAL NAMES (CNs) PRESENT FROM JANUARY 1926 TO DATE.

RECORDS LAST ADDED: 3 December 2008 (20081203/ED)

BIOSIS has been augmented with 1.8 million archival records from 1926 through 1968. These records have been re-indexed to match current BIOSIS indexing.

FILE EMBASE

FILE COVERS 1974 TO 3 Dec 2008 (20081203/ED)

EMBASE was reloaded on March 30, 2008.

EMBASE is now updated daily. SDI frequency remains weekly (default) and biweekly.

This file contains CAS Registry Numbers for easy and accurate substance identification.

Beginning January 2008, Elsevier will no longer provide EMTREE codes as part of the EMTREE thesaurus in EMBASE. Please update your current-awareness alerts (SDIs) if they contain EMTREE codes.

For further assistance, please contact your local helpdesk.

FILE PASCAL
FILE LAST UPDATED: 1 DEC 2008 <20081201/UP>
FILE COVERS 1977 TO DATE.

>>> SIMULTANEOUS LEFT AND RIGHT TRUNCATION IS AVAILABLE
IN THE BASIC INDEX (/BI) FIELD <<<

FILE CABA
FILE COVERS 1973 TO 6 Nov 2008 (20081106/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

The CABA file was reloaded 7 December 2003. Enter HELP RLOAD for details.

FILE CEABA-VTB
FILE LAST UPDATED: 17 NOV 2008 <20081117/UP>
FILE COVERS 1966 TO DATE

>>> DECHEMA, the producer of CEABA-VTB is using a new classification scheme.
The new classification schemes are available as a PDF file and may be downloaded free-of-charge from:
<http://www.stn-international.de/news/cc-de.pdf>
and
<http://www.stn-international.de/news/cc-en.pdf> <<<

FILE LIFESCI
FILE COVERS 1978 TO 13 Nov 2008 (20081113/ED)

FILE BIOENG
FILE LAST UPDATED: 27 OCT 2008 <20081027/UP>
FILE COVERS 1982 TO DATE

>>> SIMULTANEOUS LEFT AND RIGHT TRUNCATION AVAILABLE IN
THE BASIC INDEX <<<

FILE BIOTECHNO
FILE LAST UPDATED: 7 JAN 2004 <20040107/UP>
FILE COVERS 1980 TO 2003.
THIS FILE IS A STATIC FILE WITH NO UPDATES

>>> SIMULTANEOUS LEFT AND RIGHT TRUNCATION AVAILABLE IN
/CT AND BASIC INDEX <<<

FILE BIOTECHDS
FILE LAST UPDATED: 1 DEC 2008 <20081201/UP>
FILE COVERS 1982 TO DATE

>>> USE OF THIS FILE IS LIMITED TO BIOTECH SUBSCRIBERS <<<

FILE DRUGU
FILE LAST UPDATED: 1 DEC 2008 <20081201/UP>
>>> DERWENT DRUG FILE (SUBSCRIBER) <<<

>>> FILE COVERS 1983 TO DATE <<<
>>> THESAURUS AVAILABLE IN /CT <<<

FILE DRUGB
>>> FILE COVERS 1964 TO 1982 - CLOSED FILE <<<

FILE VETU
FILE LAST UPDATED: 2 JAN 2002 <20020102/UP>
FILE COVERS 1983-2001

FILE VETB
FILE LAST UPDATED: 25 SEP 94 <940925/UP>
FILE COVERS 1968-1982

FILE SCISEARCH

FILE COVERS 1974 TO 27 Nov 2008 (20081127/ED)

SCISEARCH has been reloaded, see HELP RLOAD for details.

FILE CONFSCI
FILE COVERS 1973 TO 6 Nov 2008 (20081106/ED)

CSA has resumed updates, see NEWS FILE

FILE DISSABS
FILE COVERS 1861 TO 24 OCT 2008 (20081024/ED)

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FILE RDISCLOSURE
FILE LAST UPDATED: 12 NOV 2008 <20081112/UP>
FILE COVERS 1960 TO DATE

>>> SIMULTANEOUS LEFT AND RIGHT TRUNCATION IS AVAILABLE IN THE
BASIC INDEX (/BI) AND TITLE (/TI) FIELDS <<<

10/772,445

>>> IMAGES ARE AVAILABLE ONLINE AND FOR EMAIL-PRINTS <<<

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